CRYSTALS OF THE *ESCHERICHIA COLI* MEMBRANE-ASSOCIATED GLYCOSYLTRANSFERASE (MurG) PROTEIN, ATOMIC COORDINATES AND THREE-DIMENSIONAL STRUCTURES THEREOF, ATOMIC COORDINATES AND THREE-DIMENSIONAL STRUCTURES OF BINDING DOMAINS THEREOF, IMAGES THEREOF, AND METHODS OF CRYSTALLIZING MurG PROTEINS, MODELS OF UDP-GLYCOSYLTRANSFERASES, MurG PROTEINS AND BINDING SITES, METHODS OF MAKING MODELS, METHODS OF USING MODELS OF MurG, COMPOUNDS THAT BIND, INHIBIT OR STIMULATE MurG PROTEINS, AND THERAPEUTIC COMPOSITIONS THEREOF

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FIELD OF THE INVENTION

The present invention relates to crystals of the *Escherichia coli* MurG, a membrane-associated UDP-glycosyltransferase involved in peptidoglycan biosynthesis. The present invention also relates to three-dimensional atomic coordinates of the MurG protein, three-dimensional structures of the protein, and images thereof. The present invention also relates to the atomic coordinates and three-dimensional structures of the α-carbon backbone of the MurG protein and images thereof. The present invention further relates to the atomic coordinates and three-dimensional structures of the α-carbon backbone and conserved amino acid residue sidechains of the MurG protein and images thereof. The present invention further relates to three-dimensional atomic coordinates of the donor nucleotide binding site, the acceptor binding site, and the membrane association site of the MurG protein, three-dimensional structures of the binding domains, and images thereof. The present invention also relates to computer readable media encoded with sets of the three-dimensional coordinates of the *E. coli* MurG protein, the α-carbon backbone of the MurG protein, the α-carbon backbone and the conserved amino acid residue sidechains of the MurG protein, the donor nucleotide binding site, the acceptor binding site, and the membfane association site. The present invention relates to methods of crystallizing MurG proteins.

The present invention relates to models of three-dimensional structures of UDP-glycosyltransferases and, in particular, MurG proteins, based on the three-dimensional structure of crystals of the *Escherichia coli* MurG. The present invention also relates to models of the three-dimensional structures of the α-carbon backbone of UDP-glycosyltransferases and MurG proteins. The present invention further relates to

models of the three-dimensional structure of the α-carbon backbone and conserved amino acid residue sidechains of UDP-glycosyltransferases, in particular, MurG proteins. The present invention further relates to models of the three-dimensional structures of donor nucleotide binding sites, acceptor binding sites, and membrane association sites of UDP-glycosyltransferases, in particular, MurG proteins. The present invention also relates to methods of drug design using models of this invention. The present invention further relates to compounds identified using models of the present invention that bind, inhibit or stimulate UDP-glycosyltransferases or MurG proteins. The present invention relates to compositions comprising compounds identified using the models of this invention for therapeutic or diagnositic uses. Also, the present invention relates to methods of making models of the present invention.

BACKGROUND OF THE INVENTION

The increasing frequency of resistance to existing antibiotics represents a serious public health threat. Structural and mechanistic information on essential bacterial enzymes could lead to the development of antibiotics that are active against resistant microorganisms. Both gram positive and gram negative bacterial cells are surrounded by a cross-linked carbohydrate polymer, peptidoglycan, which protects them from rupturing under high osmotic pressures. Many of the best antibiotics function by inhibiting peptidoglycan synthesis, which ultimately causes cell lysis. In recent years, intense effort has been focused on determining the structures of the enzymes that synthesize peptidoglycan. Structures of several of the early enzymes in the biosynthetic pathway have been reported (Benson *et al.*, 1995; Bertrand *et al.*, 1997; Fan *et al.*, 1994; Skarzynski *et al.*, 1996); however, the later enzymes have proven more difficult to study because both they and their substrates are membrane-associated.

MurG is the last enzyme involved in the intracellular phase of peptidoglycan synthesis (Bugg & Walsh, 1993). It catalyzes the transfer of N-acetyl glucosamine (NAG) from UDP to the C4 hydroxyl of a lipid-linked N-acetylmuramoyl pentapeptide (NAM) to form a β-linked NAG-NAM disaccharide that is transported across the cell membrane where it is polymerized and cross-linked (Fig. 1). In bacterial cells MurG associates with the cytoplasmic surface of the membrane (Bupp & van Heijenoort, 1993). However, we have found that *E. coli* MurG can be solubilized at high concentrations in active form (Ha et al., 1999).

The elucidation of the protein structure of a MurG protein is of importance in the identification and formulation of anti-bacterial agents. Until the discovery of the present invention, the structure and resulting mechanism by which MurG functions was not known. Thus, despite the important role of MurG in peptidoglycan synthesis, development of useful agents for treatment or diagnosis of disease was hindered by lack of structural information of the protein.

In order to obtain structural information on a MurG protein, it is important to have purified, active enzyme. The demonstration of activity requires a suitable assay, which in turn requires access to the natural substrates or analogues thereof. The study of MurG was hampered by difficulties obtaining and handling the lipid-linked NAM substrate (commonly known as Lipid I). This problem was overcome by Walker and coworkers, who developed a synthetic route to a set of substrate analogues of Lipid I that were shown to function as glycosyl acceptors in a glycosyl transfer reaction catalyzed by MurG. Some of these substrate analogues are freely water soluble, making it possible to monitor the activity of purified *E. coli* MurG in buffer in the absence of natural or artificial membranes or detergents.

The linear nucleic acid and amino acid sequences of *E. coli* MurG were reported in 1992. Subsequently, the nucleic acid and amino acid sequence of *B. subtilus* MurG was reported. Since then, many bacterial genomes have been sequenced and the information has been deposited in databases. Information based only on linear sequences, however, cannot accurately predict the three-dimensional structure of the protein and its functional domains.

Therefore, there is a need in the art to elucidate the three-dimensional structure of a MurG protein. One three-dimensional structure of a MurG protein can be used to construct models of other MurG proteins and to facilitate the structure determination of crystalline forms of other MurG proteins. Structures and models of MurG proteins can also be used to design proteins containing only the donor binding site or the acceptor binding site. These proteins can be used in assays, including NMR-based assays, to identify -- or characterize the mode of binding of -- ligands that bind in or near the vicinity of the substrates. These ligands or compounds can then be used as leads for the design of inhibitors that have therapeutic activity. Structures and models of MurG proteins can also be used in computer-based drug design.

SUMMARY OF THE INVENTION

The present invention relates to crystalline *Escherichia* coli MurG protein. Obtaining such crystals is an unexpected result. It is well known in the protein crystallographic art that obtaining crystals of quality sufficient for determining the structure of a protein is unpredictable. In particular, obtaining crystals of quality sufficient for determining the three-dimensional (3-D) structure of MurG has not been achievable until the crystallization of MurG as disclosed in the present application. As such, determination of the three-dimensional structure of MurG has not been possible until the discovery of the present invention. Additionally, until the discovery of the present invention, derivation of the three-dimensional structure and models of other MurG proteins has not been possible. The present inventors are also the first to define the three-dimensional structure and provide three-dimensional models for drug design for MurG proteins.

Accordingly, one object of the present invention is to provide crystals of sufficient quality to obtain a determination of the three-dimensional atomic coordinates and structures of MurG to high resolution, preferably to the resolution of less than 2.0 angstroms (A). The present invention also provides methods for producing crystalline MurG protein.

The value of the crystals of *E. coli* MurG protein extends beyond merely being able to obtain such crystals. The knowledge obtained concerning the MurG crystal structure, for example, has been used by the present inventors to define the heretofore unknown tertiary structure of the MurG protein and to identify the location of the glycosyl donor and glycosyl acceptor binding domains, as well as the location of the amino acid residues that are invariant in all MurG proteins. This information can be used to design inhibitors of MurG that have therapeutic utility. The atomic coordinates of *E. coli* MurG also are used to model the heretofore unknown tertiary structures of other MurG proteins having substantially related linear amino acid sequences, such as for MurG proteins from other microorganisms. It is anticipated that homology models can be constructed even from amino acid sequences with relatively low homology because the present inventors have identified the location of the invariant amino acid residues in MurG. The relative spatial orientations of such residues is expected to be conserved in all MurG proteins.

Comparison of nucleic acid and amino acid sequences of MurG proteins indicates that the linear amino acid sequences can vary significantly. Homology between MurG proteins from different microorganisms varies from less than 30% to greater than 90%, reflecting the evolutionary relationship between the organisms. The low homology between distantly related MurG homologues is not believed to reflect significantly different folded structures. It is well known that many amino acid sequences are capable of adopting the same general fold. *E. coli* MurG contains an alpha/beta folding pattern, one of the most common folds known in proteins. It is likely that all MurG homologues contain a similar alphalbeta fold despite the differences in the linear amino acid sequences. What gives these proteins their identity is not the general fold, but the specific details - i.e., the presentation of certain amino acids on the folded structure. The present inventors have identified the location in *E. coli* MurG of a set of residues that are invariant in all MurG homologues. It is to be expected that these residues would adopt a similar spatial location with respect to the folded structure in all MurG homologues. Therefore, these invariant residues, which have been selected by evolution as the critical residues for the binding and catalytic function of the protein, provide essential information on the location of the active site and on critical contacts to the substrates/products. They also serve as constraints that make it possible to, predict the three-dimensional structures even of distantly related MurG homologues. Thus, knowledge of the three-dimensional structure of the *E. coli* MurG protein has provided a starting point for investigation into the structure of all MurG proteins.

Accordingly, a object of the present invention is to provide information regarding the atomic coordinates and three-dimensional structures of (1) the MurG protein, (2) the α-carbon backbone of the MurG protein, (3) the α-carbon backbone and conserved amino acid residues of the MurG protein, (4) the donor nucleotide binding site, (5) the acceptor binding site, and (6) the membrane association site MurG proteins.

It is also an object of this invention to solve the three-dimensional structure of UDP-glycosyltransferases, in particular target NTURG proteins, and to determine their structure and/or atomic coordinates. Further, it is an object of this invention to use the structure or atomic coordinates of the *E. coli* MurG crystal to solve the structure of different MurG protein crystals, or a crystal of a mutant protein, homolog or co-complex of MurG.

The present invention relates to models of three-dimensional structures of UDP-glycosyltransferases, in particular MurG proteins, based on the atomic coordinates of crystalline *E. coli* MurG protein.

It is a further object of this invention to provide, UDP-glycosyltransferase enzyme mutants characterized by one or more different properties as compared with wild-type MurG. These properties include altered surface charge, increased stability to subunit dissociation, altered substrate specificity or higher specific activity. MurG mutants are useful to identify those amino acids that are most important for the enzymatic activity of MurG. This information, in turn, allows the design of improved inhibitors of MurG as compared with peptidic MurG inhibitors.

Another object of the present invention is to provide computer readable mediums encoded with a set of three-dimensional coordinates of the *E. coli* MurG protein, the α-carbon backbone of the MurG protein, the α-carbon backbone and conserved amino acid residues of the MurG protein, and the nucleotide donor binding site, the acceptor binding site, the membrane association site of the MurG protein.

Another embodiment of the present invention provides three-dimensional and two-dimensional computer images of the three-dimensional structure of MurG protein, the α-carbon backbone of the MurG protein, the α-carbon backbone and conserved amino acid residues of the MurG protein, and the nucleotide donor binding site, the acceptor binding site, the membrane association site of the MurG protein.

The knowledge of the three-dimensional structure of MurG also provides a means for designing proteins that have altered beneficial functions by analyzing the structure and interactions between individual amino acids of the protein. For example, the present inventors have shown that *E. coli* MurG consists of two domains separated by a cleft.

Noncovalent interactions between the two domains are not extensive. The present inventors have shown that the domains fold independently and can, therefore, be expressed independently either alone or as part of a recombinant protein containing the acceptor binding site from one MurG homologue and the donor binding site from another MurG homologue. It would be expected that the domains of other MurG proteins could also be expressed independently, either alone or as chimaeras with other

MurG domains. Independently expressed domains of the protein are useful for discovering ligands that bind to the individual domains.

The knowledge of the three-dimensional structure of *E. coli* MurG protein and models of other MurG proteins also provides a means for designing and producing compounds that regulate, inhibit or antagonize functions of the MurG protein (i.e., structure based drug design). For example, chemical compounds can be designed to block binding of UDP-GlcNAc to a MurG protein using various computer programs and models.

It is also an object of this invention to use the structure coordinates and atomic details of MurG, or its mutants or homologues or co-complexes, to design, evaluate computationally, synthesize and use inhibitors of MurG that avoid the undesirable physical and pharmacologic properties of peptidic MurG inhibitors.

Another embodiment of the present invention is a composition comprising MurG protein in a crystalline form.

Yet another embodiment of the present invention is a method for producing crystals of MurG, comprising combining MurG protein in a suitable buffer with a suitable amount of a reservoir buffer containing a detergent, and inducing crystal formation to produce said MurG crystals.

BRIEF DESCRIPTION OF THE DRAWINGS

Fig. 1. Pathway for peptidoglycan biosynthesis.

Fig. 2. Overall architecture of MurG. A. Stereo view of the MurG structure. The N domain is shown in purple; the C domain is shown in green. The figure was generated with the programs MOLSCRIPT (Klaulis, 1991) and RASTER31) (Merrit & Murphy, 1994). B. Topology diagram of MurG.

Fig. 3. Identification of critical residues in MurG and related glycosyltransferases. A. Sequence alignment of *E. coli* MurG with homologs from seven other bacterial strains, deliberately chosen to represent a disparate group of organisms. The secondary structure of *E. coli* MurG is shown above the sequences. Gaps mapping to the loop regions of *E. coli* MurG suggest that some sequences include other structural elements. Residues highlighted in blue are invariant among the eighteen MurG sequences available. Residues highlighted in yellow are identical in 85% of the eighteen homologs, while in the remaining 15%, only closely related amino

acid substitutions are found. Highly conserved residues that do not meet the stringent criteria established for highlighting are shown in the consensus sequence. A consensus motif for UDP-glucuronosyltransferases is also shown. Numbering is with respect to the overexpressed *E. coli* MurG construct, which contains an additional N-terininal methionine. B. Mapping of the G loops and other highlighted residues from Fig. 3a in red on the MurG structure. Side chains for highly conserved residues are also shown. C. Model for the proposed UDP-binding subdomain found in many UDP-glycosyltransferases based on the *E. coli* MurG structure. Conserved residues in UDP-glucuronosyltransferases are highlighted in red. Side chains are shown for residues that are located near the cleft and may be involved in substrate binding. The glutamate residue is proposed to interact with the ribose sugar. The dotted loop varies in length within the MurG family and in other UDP-sugar transferases, but the N and Q on the following helix are invariant. Note that the UDPglucuronosyltransferases contain a conserved D preceding the Q, which is not shown on this model.

Fig 4. Structural analysis of the substrate binding pockets in MurG. A. Structural comparison between the C-terminal domain of phage T4 β-glucosyltransferase (left) and the C-terminal domain of *E. coli* MurG (right). The aligned six β-strands are magenta, the aligned α-helices are orange, and the other structural elements are blue. In β-glucosyltransferase, key residues involved in UDP binding are highlighted in yellow. The analogous residues in MurG are also highlighted in yellow. B. A close-up view of the proposed donor binding pocket in the MurG C domain with the docked UDP-GlcNAc. Conserved residues in MurG are colored magenta. The carbonyl oxygen of residue 1245 is shown in red, and its backbone nitrogen is shown in blue. C. The surface of *E. coli* MurG. The G loops and other conserved residues in MurG are colored magenta. The proposed membrane binding interface is also highlighted with hydrophobic residues in yellow and positively charged residues in blue.

DEFINITIONS

It is to be noted that the term "a" or "an" entity refers to one or more of that entity; for example, a compound refers to one or more compounds or at least one compound. As such, the terms "a" (or "an"), "one or more", and "at least one" can be used interchangeably herein.

It is also to be noted that the terms "comprising", "including" and "having" can be used interchangeably. Furthermore, a compound "selected from the group consisting of" refers to one or more of the compounds in the list that follows, including mixtures (i.e., combinations) of two or more of the compounds.

According to the present invention, an isolated, or pure, protein, is a protein that has been removed form its natural milieu. As such, "isolated" and "biologically pure" do not necessarily reflect the extent to which the protein has been purified. An isolated protein of the present invention can be obtained from its natural source, can be produced using recombinant DNA technology or can be produced by chemical synthesis.

It is also to be noted that the terms "tertiary" and "three-dimensional" can be used interchangeably.

It is also to be noted that reference to a "MurG protein" can also be recited as "MurG" and such terms can be used to refer to the complete MurG protein, a portion of the MurG protein, such as a polypeptide.

The following terms are also used herein:

The term "naturally occurring amino acids" means the L-isomers of the naturally occurring amino acids. The naturally occurring amino acids are glycine, alanine, valine, leucine, isoleucine, serine, methionine, threonine, phenylalanine, tyrosine, tryptophan, cysteine, proline, histidine, aspartic acid, asparagine, glutamic acid, glutamine, gamma-carboxyglutamic acid, arginine, ornithine and lysine. Unless specifically indicated, all amino acids referred to in this application are in the L-form.

The terin "unnatural amino acids" means amino acids that are not naturally found in proteins. Examples of unnatural amino acids used herein, include racemic mixtures of selenocysteine and selenomethionine. In addition, unnatural amino acids include the D or L forms of nor-leucine, para-nitrophenylalanine, homophenylalanine, parafluorophenylalanine, 3-amino-p2-benzylpropionic acid, homoarginine, and D-phenylalanine.

The term "positively charged amino acid" includes any naturally occurring or unnatural amino acid having a positively charged side chain under normal physiological conditions. Examples of positively charged naturally occurring amino acids are arginine, lysine and histidine.

The term "negatively charged amino acid" includes any naturally occurring or unnatural amino acid having a negatively charged side chain under normal physiological conditions. Examples of negatively charged naturally occurring amino acids are aspartic acid and glutamic acid.

The term "hydrophobic amino acid" means any amino acid having an uncharged, nonpolar side chain that is relatively insoluble in water. Examples of naturally occurring hydrophobic amino acids are alanine, leucine, isoleucine, valine, proline, phenylalanine, tryptophan and methionine.

The term "hydrophilic amino acid" means any amino acid having an uncharged, polar side chain that is relatively soluble in water. Examples of naturally occurring hydrophilic amino acids are serine, threonine, tyrosine, asparagine, glutamine, and cysteine.

The term "MurG" refers to a UDP-glycosyltransferase that has a two domain strucuture, where each domain contains a set of invariant residues as shown in Fig. 3a, including any mutant, homologue or co-complex or any similar enzyme that catalyzes the transfer of N-acetylglucosamine (GlcNAc) from UDP to the C4 hydroxyl of the lipidlinked MurNAc pentapeptide.

The term "mutant" refers to a MurG polypeptide, i.e., a polypeptide displaying the biological activity of a wild-type MurG, characterized by the replacement of at least one amino acid from the wild-type, *E. coli* MurG sequence according to Ikeda, et al., Nucleic Acids Res. 1990, and Mengin-LeCreuix et al., Nucleic Acids Res. 1990. Such a mutant may be prepared, for example, by expression of MurG cDNA previously altered in its coding sequence by PCR-based mutagenesis method.

MurG mutants may also be generated by site-specific incorporation of unnatural amino acids into MurG proteins using the general biosynthetic method of Noren, C. J., et al., Science, 244, pp.182-188 (1989). In this method, the codon encoding the amino acid of interest in wild-type MurG is replaced by a "blank" nonsense codon, TAG, using oligonucleotide-directed mutagenesis (described in detail, infra). A suppressor tRNA directed against this codon is then chemically aminoacylated in vitro with the desired unnatural amino acid. The aminoacylated tRNA is then added to an in vitro translation system to yield a mutant MurG enzyme with the site-specific incorporated unnatural amino acid.

Selenocysteine or selenomethionine may be incorporated into wild-type or mutant MurG by expression of MurG-encoding cDNAs in auxotrophic *E. coli* strains. Hendrickson, W. A. et al., EMBO J., 9(5), pp. 1665-1672 (1990). In this method, the wild-type or mutagenized MurG CDNA may be expressed in a host organism on a growth medium depleted of either natural cysteine or methionine (or both) but enriched in selenocysteine or selenomethionine (or both).

The term "altered surface charge" means a change in one or more of the charge units of a mutant polypeptide, at physiological pH, as compared to wild-type MurG. This is preferably achieved by mutation of at least one amino acid of wild-type MurG to an amino acid comprising a side chain with a different charge at physiological pH than the original wild-type side chain.

The change in surface charge is determined by measuring the isoelectric point (pI) of the polypeptide molecule containing the substituted amino acid and comparing it to the isoelectric point of the wild-type MurG molecule.

The term "altered substrate specificity" refers to a change in the ability of a mutant MurG to cleave a substrate as compared to wild-type MurG.

The "kinetic form" of MurG refers to the condition of the enzyme in its free or unbound form or bound to a chemical entity at either its active site or accessory binding site.

A "competitive" inhibitor is one that inhibits MurG activity by binding to the same kinetic form of MurG as its substrate binds—thus directly competing with the substrate for the active site of MurG. Competitive inhibition can be reversed completely by increasing the substrate concentration.

An "uncompetitive" inhibitor is one that inhibits MurG by binding to a different kinetic form of the enzyme than does the substrate. Such inhibitors bind to MurG already bound with the substrate and not to the free enzyme. Uncompetitive inhibition cannot be reversed completely by increasing the substrate concentration.

A "non-competitive" inhibitor is one that can bind to either the free or substrate bound form of MurG.

Those of skill in the art may identify inhibitors as competitive, uncompetitive or non-competitive, by computer fitting enzyme kinetic data using standard equations according to Segel, I. H., Enzvme Kinetics, J. Wiley & Sons, (1975). It should also be

understood that uncompetitive or non-competitive inhibitors apcording to this invention may bind to the accessory binding site.

The term "homolog" means a protein having at least 25% amino acid sequence identity with MurG or any functional part of MurG, and including certain invariant amino acid residues corresponding to G14, G15, G18, H19, G104, H124, E125, G190, G191, S192, G194, A195, R261, G263, A264, E269, P281, Q289, N292 and A293 (as numbered in the E.coli MurG sequence set forth in Fig. 3a) and also including three glycine rich loops. A homolog may contain some or all of the invariant residues.

The term "co-complex" means MurG or a mutant or homologue of MurG in covalent or non-covalent association with a chemical entity or compound.

The term "associating with" refers to a condition of proximity between a chemical entity or compound, or portions thereof, and a MurG molecule or portions thereof. The association may be non-covalent--wherein the juxtaposition is energetically favored by hydrogen bonding or van der Waals or electrostatic interactions--or it may be covalent.

The term ".beta.-sheet" refers to the conformation of a polypeptide chain stretched into an extended zig-zig conformation. Portions of polypeptide chains that run "parallel" all run in the same direction. Polypeptide chains that are "antiparallel" run in the opposite direction from the parallel chains.

The terms "atomic coordinates" or "structure coordinates" refer to mathematical coordinates derived from mathematical equations related to the patterns obtained on diffraction of a monochromatic beam of X-rays by the atoms (scattering centers) of a MurG molecule in crystal form. The diffraction data are used to calculate an electron density map of the repeating unit of the crystal. The electron density maps are used to establish the positions of the individual atoms within the unit cell of the crystal.

The term "heavy atom derivatization" refers to the method of producing a chemically modified form of a crystal of MurG. In practice, a MurG crystal is soaked in a solution containing heavy metal atom salts, or organometallic compounds, e.g., lead chloride, gold thiomalate, thimerosal, uranyl acetate or mercuric chloride, which can diffuse through the crystal and bind to the surface of the protein. The location(s) of the bound heavy metal atom(s) can be deetermined by X-ray diffraction analysis of the soaked crystal. This information, in turn, is used to generate the phase information used

to construct three-dimensional structure of the enzyme. Blundel, T. L. and N. L. Johnson, Protein Crystallography, Academic Press (1976).

Those of skill in the art understand that a set of structure coordinates determined by X-ray crystallography is not without standard error. For the purpose of this invention, any set of structure coordinates for MurG or MurG homologues or MurG mutants that have a root mean square deviation of protein backbone atoms (N, C.alpha., C and 0) of less than 0.75 Å when superimposed--using backbone atoms--on the structure coordinates listed in Table 1, Table 2 or Table 3 shall be considered identical.

The term "unit cell" refers to a basic parallelepiped shaped block. The entire volume of a crystal may be constructed by regular assembly of such blocks. Each unit cell comprises a complete representation of the unit of pattern, the repetition of which builds up the crystal.

The term "space group" refers to the arrangement of symmetry elements of a crystal.

The term "molecular replacement" refers to a method that involves generating a preliminary model of a MurG crystal whose structure coordinates are unknown, by orienting and positioning a molecule whose structure coordinates are known (e.g., MurG coordinates from Table 1, 2, or 3) within the unit cell of the unknown crystal so as best to account for the observed diffraction pattern of the unknown crystal. Phases can then be calculated from this model and combined with the observed amplitudes to give an approximate Fourier synthesis of the structure whose coordinates are unknown. This, in tum, can be subject to any of the several forms of refinement to provide a final, accurate structure of the unknown crystal. Lattman, K., "Use of the Rotation and Translation Functions", in Methods in Enzymology, 115, pp. 55-77 (1985); M. G. Rossmann, ed., "The Molecular Replacement Method", Int. Sci. Rev. Ser., No. 13, Gordon & Breach, New York, (1972). Using the structure coordinates of MurG provided by this invention, molecular replacement may be used to determine the structure coordinates of a crystalline mutant or homologue of MurG or of a different crystal form of MurG.

DETAILED DESCRIPTION OF THE INVENTION

The present invention relates to the discovery of the three-dimensional structure of the crystalline form of the *E. coli* MurG protein, models of such three-dimensional

structures, a method of structure based drug design using such structures, methods to identify ligands or compounds that interact or bind with such structures, the compounds identified by such methods, and the use of such compounds in therapeutic compositions.

More particularly, the present invention relates to novel crystals of *E. coli* MurG protein, methods of production of such crystals, three-dimensional coordinates of MurG protein, MurG structures and models derived from the *E. coli* MurG structure, and uses of such structures and models to derive other MurG structures and in ligand discovery and drug design strategies.

The present invention also relates to three-dimensional structures and coordinates of the donor nucleotide binding site, the acceptor binding site, and the membrane association site of the MurG protein, structures and models of the binding sites, and uses of such structures and models to derive the binding sites of other MurG proteins and in drug design strategies.

Solely for ease of explanation, the description of the invention is divided into the following sections: (1) crystals of MurG protein; (2) methods of crystallization; (3) three-dimensional crystal coordinates and structure of *E. coli* MurG; (4) three-dimensional coordinates and structure of the donor nucleotide binding site of MurG; (5) coordinates and structure of the acceptor binding site of MurG; (5) three-dimensional coordinates and structure of the membrane association site; (6) two-dimensional and three-dimensional images of the protein, α-carbon backbone, α-carbon backbone with conserved amino acid residues, and binding sites; and (7) computer readable mediums comprising the three-dimensional coordinates of the MurG protein, α-carbon backbone, α-carbon backbone with conserved amino acid residues, and binding sites; (8) images of structures of MurG protiensand binding sites; (9) models of MurG proteins and binding sites thereof and methods of using the structure of MurG to determine the structures of other MurG proteins and binding sites; (10) structure based drug design using models of MurG protein and binding site structures; (11) compounds derived from structure based drug design; and (12) therapeutic compositions using drugs designed from structure based drug design.

CRYSTALS

One embodiment of the present invention includes a pomposition comprising a MurG protein in a crystalline form (i.e., MurG crystals). As used herein, the terms (crystalline MurG" and "MurG crystal" both refer to crystallized MurG protein and are intended to be used interchangeably. More particularly, an embodiment of the present invention includes a composition comprising an *E. coli* MurG protein in a crystalline form. Preferably, a crystalline MurG is produced using the crystal formation method described herein, in particular according to the method disclosed in Example 1. A MurG crystal of the present invention comprises any crystal structure and preferably precipitates as a triclinic crystal. Preferably, a composition of the present invention includes MurG crystal molecules arranged in a crystalline manner in a P1 space group with two molecules per assymmetric unit so as to form a unit cell of dimensions a=60.613 Å, b=66.356 Å, c=67.902 Å, α=64.294, β=83.520, γ=65.448. A preferred crystal of the present invention provides X-ray diffraction data for determination of atomic coordinates to a resolution of about 3.0 Å, preferably to about 2.4 Å, and more preferably to about 1.8 Å.

Another embodiment of the present invention includes crystalline MurG protein co-crystallized with a donor nucleotide or substrate or substrate analog. Preferably, a donor nucleotide is UDP or UDP-GlcNAc (UDP-N-acetylglucosamine) or an analog thereof. The substrate or substrate analog is preferably Lipid I or Lipid II or analogs of Lipid I or Lipid II. More specifically, Lipid I and II analogs are as described in PCT/US99/02187, published as W099/38958 and US Provisional Application Nos. 60/122,966 filed March 3, 1999 and 60/137,696 filed June 4, 1999, and International Application No. PCT/US00/05554 entitled "Bacterial transglycosylases: Assays for monitoring the activity using Lipid II substrate analogs and methods for discovering antibiotics," all incorporated herein by reference in their entirety.

Included in the present invention, a variety of MurG proteins from numerous organisms can be used to prepare MurG crystals, including but not limited to, microorganisms such as bacteria, higher-order bacteria, thermal stable bacteria, spirochetes, small pathogenic organisms, fungi, protozoa, cyanobacteria, and trypanosomes. More particularly, bacteria such as but not limited to, *Escherichia coli, Bacillus subtilis, Aquefe-x aeolicus, Borrelia burgdorferi, Chlamydia pneumoniae, Chlamydia trachomatis, Enterococcus jaecais, Enterococcus hirae, Haemophilus*

influenzae, Helicobacter pylori J99, Helicobacter pylori, Mjrobacterium tuberculosis, Porphyromonas gingivalis, Rickettsia prowazekii, Streptomyces coelicolor, Streptomyces collinus, Streptococcus pneumoniae, Synechocystis sp. (strain PCC6803), *Thermotoga maritime,* and *Treponemapallidum.*

In another embodiment of the present invention, the MurG proteins or fragments thereof, mutants or homologs are expressed in, for example, an *E. coli* host cell for use expressing sufficient quantities of sufficiently purified protein to form crystals. The present inventors have demonstrated that it is possible to express *Enterococcus. jaecalis* MurG in *E. coli* cells - so the MurG proteins from many organisms can be cloned into expression vectors suitable for expression in *E. coli* cells. This would facilitate obtaining sufficient quanitites of isolated or purified MurG proteins. The expression of E. *jaecalis* MurG protein in *E. coli* host cells is performed, for example, by expressing the E. *jaecalis* MurG gene cloned into a pET21b expression vector and transformed into an *E. coli* host cell. The MurG protein is over-expressed with a C-terminal his tag (LEHHHHHH) which allows the protein to be purified using a His-tag affinity column. The protein is then crystallized and the atomic coordinates are determined using X-ray diffraction and methods known to those skilled in the art.

It is another embodiment of the present invention to provide for the construction and expression of chimaeric MurG proteins to enable the crystallization and determination of the three-dimensional coordinates of such chimeras. For example, if there are problems obtaining or crystallizing MurGs from other organisms, the present invention provides information that makes it possible to make chimaeric proteins containing the donor or acceptor binding site from *E. coli* MurG and the corresponding acceptor or donor binding site from another organism. Chimaeric proteins could be easier to express, handle, or crystallize. For example, we have found that E. faecalis MurG is more difficult to solubilize that *E. coli* MurG (requiring more detergent). It is believed that the problems are related to the acceptor binding domain having a stronger affinity for the bacterial membranes. To overcome this problem, one can attach the donor binding domain of *E. faecalis* to the *E. coli* acceptor binding site and determine structure to see details of *E. faecalis* donor binding domain.

According to the present invention, crystalline MurG can be used to determine the ability of a chemical compound to bind to a MurG protein in a manner predicted by

a structure based drug design method of the present invention. Preferably, a MurG crystal is soaked in a solution containing a chemical compound of the present invention. Binding of the chemical compound to the crystal is then determined by methods standard in the art. Thereby, the co-crystal of MurG and a compound of interest is determined.

METHODS OF CRYSTALLIZATION

The present invention includes a method for producing crystals of MurG proteins, comprising: combining MurG protein with a reservoir solution and inducing crystal formation to produce MurG crystals. Another embodiment of the present invention, a method for producing crystals of MurG protein comprises combining MurG protein with UDP-GlcNAc in a 1:3 ratio and with a reservoir solution and inducing crystal formation to produce MurG crystals.

Preferably, crystals of MurG are formed using a solution containing a range of MurG protein from about 1 mg/ml to about 20 mg/ml, more preferably above 5 mg/ml, limited only by the solubility of the protein, which may vary depending on the specific amino acid sequence.

A reservoir solution contains the buffer, the precipitant, and additives if necessary. A suitable reservoir buffer of the present invention comprises NaMES (2-[N-morpho]inolethanesulfonic acid, sodium salt) buffer, NaHEPES (N-[2-hydroxyethyl]piperazine-N'-[2-ethanesulfonic acid, sodium salt) buffer, Tris (tris[hydroxymethyl]aminomethane) buffer, and any buffer which has the PKa between 5.5 and 8.0. A suitable NaMES buffer solution has a pH range from about 5.6-6.5. Most preferably, the NaMES buffer has a pH of about 6.5. The precipitant comprises ammonium sulfate, saturated sodium and potassium tartrate and polyethylene glycol. A suitable concentration of ammonium sulfate can range from 0.8 M to 1.5 M. Most preferably, the ammonium sulfate concentration is about 0.96 M. A suitable additive comprises detergents like Triton X-100 and n-octyl-beta-glucoside. The concentration of Triton X-100 can range from 0.1% to 1%. Most preferably, the concentration of Triton X-100 is 0.4%.

In a preferred embodiment, MurG crystals are produced by a method comprising concentrating MurG protein in a buffer solution, mixing the protein concentrate with

UDP-GlcNAc in a 1:3 molar ratio, mixing equal volumes of protein solution with a reservoir solution, and inducing crystal formation to produce MurG crystals.

In a particular embodiment of the invention, MurG crystals are produced by a method comprising concentrating MurG protein to 10 mg/ml in a buffer of 20 mM Tris-HCl, pH 7.9/150mM NaCl and 50 mM EDTA; mixing the protein concentrate with UDP-GlcNAc in a 1:3 molar ratio; mixing equal volumes of protein solution with a reservoir solution comprising (0.1 M NaMES, pH 6.5, 0.96 M $(NH_4),SO_4$, 0.4% TRITON® X-100, and 10 mM dithiolthreitol (DTT)), and inducing crystal formation using hanging drop vapor-diffusion. This preferred method is described in greater detail in Example 1.

Supersaturated solutions of MurG protein can be induced to crystallize by several methods including, but not limited to, vapor diffusion, liquid diffusion, batch crystallization, constant temperature and temperature induction or a combination thereof. Preferably, supersaturated solutions of MurG protein are induced to crystallize by vapor diffusion (i.e., hanging drop method). In a vapor diffusion method, a MurG protein solution is combined with a reservoir solution of the present invention that will cause the MurG protein solution to become supersaturated and form MurG crystals at a constant temperature. Vapor diffusion is preferably performed under a controlled temperature in the range of from about 15° C to about 30° C, more preferably from about 20° C to about 25° C, and most preferably at a constant temperature of about 22° C.

In another preferred embodiment, the present invention includes a method to produce crystals of MurG protein comprising the steps of: (a) preparing an about 10 mg/ml solution of MurG protein in a Tris-HCI buffer, (mixing UDP-GlcNAc with the Mur-G protein solution in a 3:1 molar ratio, (c) dropping 2 µl droplet of this protein sample onto a coverslip, (d) adding an equal volume of reservoir solution to this droplet and inverting this over a well containing about 1 ml of the reservoir solution; and (e) incubating until crystals of MurG form.

Any isolated MurG protein can be used with the present method. An isolated MurG protein can be isolated from its natural milieu or produced using recombinant DNA technology (e.g., polymerase chain reaction (PCR) amplification, cloning) or chemical synthesis. To produce recombinant MurG protein, a nucleic acid molecule

encoding a MurG protein can be inserted into any vector capable of expressing the nucleic acid in a host clell. Suitable and preferred nucleic acid molecules to include in recombinant vectors of the present invention are as disclosed herein. Such suitable and preferred nucleic acid molecules include numerous MurG encoding genes that have been isolated to date, and that will be isolated in the future. A preferred nucleic acid molecule of the present invention encodes a homologue of MurG. Homologues of MurG can be recognized by the presence of certain conserved amino acid residues or sequences.

A sequence alignment for six MurG sequences is shown in Fig. 3A. Highlighted residues include those that are invariant or almost invariant across all MurG proteins. A nucleic acid molecule of the present invention can encode any portion of a MurG protein, preferably a full-length MurG protein or either of the two domains. A more preferred nucleic acid molecule to include in a recombinant vector, and particularly in a recombinant molecule, includes a nucleic acid molecule encoding a protein having the amino acid sequence represented by amino acid sequences of MurG proteins as deposited in the NCBI database and are identified with Accession Nos. CAB51993, A71316, E70579, C71699, F70195, A43727, JC1275, BVECMG, CEECAM, O83535, Q9ZK59, CAB85280, AAF39020, BAA18775, AAD26629, CAB73295, P37585, Q9ZHA9, Q9ZHDC0, Q9ZBA5, Q9X4H4, Q9WY74, P74657, O06224, Q9Z702, O84766, O69552, O67238, O51708, O25770, O07670, O07109, P45065, CAB66324, AAC68356, AAF06830, P18579, P17443, P17952, P16457, P07862, AAE23178, AAD53936, CAA18668, CAA38869, CAA38868, CAA38867, CAA38866, AAD08196, BAA01453, BAA01455, BAA01454, AAD19042, CAA45558, CAA74235, AAD10537, AAD06652, AAC95450, CAA14869, AAC73201, AAC65509, AAC67113, AAC45636, CAB08640, AAC22793, AAC07193, BAA24357, CAB13395, BAA01355, AAB35538, 1904153C, 1808265B, 1808265A, CAA36866, CAA36869, CAA36868, CAA36867, CAA36776, and AAA99436. Further, examples of nucleic acid molecules encoding MurG proteins have been deposited in NCBI, Genbank, and have Accession Nos. AL162758, AE002281, D90917, AF110367, AL139077, AJ242646, AE000520, AE000511, L42023, U00096, NC-000922, AE000783, AE000657, AE001348, AF099188, AR048673, AR048672, AF179611, AL022602, AL109663, X55034, AE000621,

D10602, AE001670, X64259, Y13922, U10879, AE001535, AF068902, AJ235271, AE000118, AE001227, AE001176, U94707, Z95388, U32793, AE000727, D84504, Z99111, D10483, X52644, X52540, and L24773. These sequences are known and are publicly available. Further, as additional genomes and genes are sequenced, more MurG encoding nucleotide sequences will become available, and can be used in the present invention.

In specific embodiments of the invention, the protein sequence of *E. coli* MurG was reported in 1990 (Ikeda et al. Nucleic Acids Res. 1990, 19:4014; and Mengin-Lecreuix, D. et al., Nucleic Acids Res. 1990, 18:2810.). *E. coli* genomic DNA can be purified from *E. coli* or purchased from ATCC, or the gene for *E. coli* MurG is cloned into a plasmid can be obtained from numerous sources. Primers were designed to the portions of the gene corresponding to the N and C termini of the protein. The primers also encoded restriction enzyme sites outside the protein coding region. The gene sequence was amplified; the corresponding double stranded nucleic acid molecule was cut with appropriate restriction enzymes for cloning into a commercially available expression vector (pET expression vectors available from Novagen provide for numerous variations of MurG protein - wild-type or fusion proteins or proteins with affinity tags at N or C terminus. We have worked with several constructs but found that MurG with a His-tag at C-terminus crystallized best; the protein sequence contained an extra methionine at N-terminus and eight extra residues at C terminus, six of which were histidines. The vector used was pET21b. (as described in Ha et al. J. Am. Chem. Soc. 121, (1999) 8415-8426 hereby incorporated by reference in its entirety).

A recombinant vector of the present invention can be either RNA (probably not) or DNA, and typically includes, but is not limited to, a virus or plasmid. Any recombinant vector and host cell that provides for expression of a MurG protein encoding mucleic acid sequence can be used in the present invention to express MurG protein for crystallization. Preferred vectors are engineered for high level expression in *E. coli* such as, but not limited to, pET vectors. We have found that over-expression of MurG from either *E. coli* or *E. faecalis* in *E. coli* cells is not toxic and, thus, this approach will work for other MurG proteins.

As used herein, an expression vector is a DNA vector that is capable of transforming a host cell and of affecting expression of a specified nucleic acid

molecule. Expression vectors of the present invention include any vectors that function (i.e., direct gene expression) in recombinant cells of the present invention, including bacterial, fungal, and other microorganisms cells. Preferred expression vectors of the present invention direct expression in bacterial cells from a plasmid. A preferred recombinant molecule of the present invention comprises pET21b with *E. coli* MurG gene cloned into the Nde 1 and Xho 1 sites.

An expression vector of the present invention can be transformed into any suitable host cell to form a recombinant cell. A suitable host cell includes any cell capable of expressing a nucleic acid molecule inserted into the expression vector. For example, a procaryotic expression vector can be transformed into a bacterial host cell. If the expression vector contains a T7 promoter then a source of T7 RNA polymerase must be provided to induce expression. Some host cells contain the T7 RNA polymerase gene in a repressed state. Expression of T7 RNA polymerase can be induced with a chemical signal such as IPTG or heat. Alternatively, a source of T7 RNA polymerase can be introduced at the appropriate time by infection with a phage containing a copy of T7 RNA polymerase. A wide range of hosts strains can be infected with a suitable phage. Some host strains have been engineered to contain inducible copies of T7 RNA polymerase gene. Such host strains include BL21(DE3) and derivatives thereof. A preferred host strain of the present invention is BL21(DE3)pLysS or BL21(DE3)pLysE, which are commercially available from Novagen and can be readily transformed with a DNA plasmid vector containing a MurG gene under the control of the T7 promoter. As already stated above, a preferred vector is a pET vector, preferably containing a restriction enzyme site permitting cloning of the gene as a fusion containing a C-terminal his tag.

In a preferred embodiment, one method to isolate MurG protein useful for producing MurG crystals includes recovery of MurG protein having a C-terminal LEHHHHHH (His tag) sequence purified as described in Ha et al. (1999, J. Amer. Chem. Soc. 121:8415-8426). One of skill in the art is able to modify this procedure in order to purify other proteins can be produced as C-terminal histadine (his) tags. The purification conditions for specific MurG proteins will vary depending upon the particular characteristics of the proteins such as their isoelectric point, molecular weight, etc. It is known that the isoelectric points of different MurG homologues vary a

bit, although they are generally relatively high. Also, some MurG homologues may be more hydrophobic than others, which will mean differences in amount of detergent necessary for purification. It is likely that all the MurG homologues can be purified over nickel affinity columns using the C-terminal his-tag as a handle. Those skilled in the art of protein purification will know how to modify purification parameters depending upon the protein characteristics, in order to purify the protein for crystallization.

STRUCTURE OF MurG PROTEIN

One embodiment of the present invention includes a model of a MurG protein, in which the model represents a three-dimensional structure of a MurG protein. Another embodiment of the present invention includes the three-dimensional structure of a MurG protein. A three-dimensional structure of a MurG protein encompassed by the present invention substantially conforms with the atomic coordinates represented in Table 1. According to the present invention, the use of the term "substantially conforms" refers to at least a portion of a three-dimensional structure of a MurG protein which is sufficiently spatially similar to at least a portion of a specified three-dimensional configuration of a particular set of atomic coordinates (e.g., those represented by Table 1) to allow the three-dimensional structure of another MurG protein to be modeled or calculated using the particular set of atomic coordinates defining the three-dimensional configuration of the MurG protein. For example, but not meant to be a limitation, homology modeling can be done using the linear sequence of a different MurG and *E. coli* coordinates; molecular replacement can allow the solution of a different MurG structure using the *E. coli* MurG coordinates and experimental data such as x-ray diffraction pattern from a different MurG crystal. According to the present invention, a three-dimensional structure of a given portion or chain of a first MurG protein can substantially conform to at least a portion of the atomic coordinates which represent a three-dimensional configuration of a second MurG.

More particularly, a structure that substantially conforms to a given set of atomic coordinates is a structure wherein at least about 50% of such structure has an average root-mean-square deviation (RMSD) of less than about 2.5 Å for the α-carbon or C-alpha backbone atoms in secondary structure elements in each domain, and more

preferably, less than about 2.0 Å for the C-alpha backbone atoms in secondary structure elements in each domain, and, in increasing preference, less than about 1.5 Å, less than about 1.0 Å, less than about 0.7 Å, and more preferably, less than about 0.5 Å for the C-alpha backbone atoms in secondary structure elements in each domain. In a more preferred embodiment, a structure that substantially conforms to a given set of atomic coordinates is a structure wherein at least about 75% of such structure has the recited average root-mean-square deviation (RMSD) value, and more preferably, at least about 90% of such structure has the recited average RMSD value, and most preferably, about 100% of such structure has the recited average RMSD value.

In an even more preferred embodiment, the above definition of "substantially conforms" can be extended to include atoms of amino acid side chains. As used herein, the phrase "common amino acid side chains" refers to amino acid side chains that are common to both the structure which substantially conforms to a given set of atomic coordinates and the structure that is actually represented by such atomic coordinates. Preferably, a three-dimensional structure that substantially conforms to a given set of atomic coordinates is a structure wherein at least about 50% of the common amino acid side chains have an average RMSD value of less than about 1.5 Å, and more preferably, less than about 1.3 Å, and in increasing preference, less than about 1.0 Å, less than about 0.7 Å, and most preferably, less than about 0.3 Å.

In a more preferred embodiment, a structure that substantially conforms to a given set of atomic coordinates is a structure wherein at least about 75% of the common amino acid side chains have the recited average RMSD value, and more preferably, at least about 90% of the common amino acid side chains have the recited average RMSD value, and most preferably, about 100% of the common amino acid side chains have the recited average RMSD value.

In more preferred embodiments of the present invention, a large number of different "rotamers" or "rotational isomers" of the MurG protein are encompassed by three-dimensional structures of the invention in which the amino acid side chains are at a variety of positions in crystalline forms of the protein or for the protein in solution. Different rotamers refer to molecules of identical configuration may be distinguished as having different conformations after rotation about the various molecular bonds. Therefore, while the same or similar amino acids may be present, the exact location will

vary depending upon the freedom of rotation of the bonds due to hydrogen bonding, and other molecular forces.

STRUCTURE OF THE α-CARBON BACKBONE OF MurG AND THE α-CARBON BACKBONE AND CONSERVED AMINO ACID RESIDUES

The present invention includes the three-dimensional structure of the α-carbon or C-alpha backbone of a MurG protein, in particular the *E. coli* MurG protein. A three-dimensional structure of the C-alpha backbone of the MurG protein encompassed by the present invention substantially conforms with the atomic coordinates represented in Table 2.

More particularly, a structure that substantially conforms to a given set of atomic coordinates is a structure wherein at least about 50% of such structure has an average root-mean-square deviation (RMSD) of less than about 2.5 Å for the C-alpha backbone atoms in secondary structure elements in each domain, and more preferably, less than about 2.0 Å for the C-alpha backbone atoms in secondary structure elements in each domain, and, in increasing preference, less than about 1.5 Å, less than about 1.0 Å, less than about 0.7 Å, and more preferably, less than about 0.5 Å for the C-alpha backbone atoms in secondary structure elements in each domain. In a more preferred embodiment, a structure that substantially conforms to a given set of atomic coordinates is a structure wherein at least about 75% of such structure has the recited average root-mean-square deviation (RMSD) value, and more preferably, at least about 90% of such structure has the recited average RMSD value, and most preferably, about 100% of such structure has the recited average RMSD value. The C-alpha backbone of MurG proteins is expected to be more conserved than the location of the particular amino acid residue side chains.

The present invention also includes the three-dimensional structure of the (α-carbon or C-alpha backbone and conserved or invariant amino acid residue side chains of a MurG protein, in particular the *E. coli* MurG protein. A three-dimensional structure of the C-alpha backbone and conserved amino acid residues of the MurG protein encompassed by the present invention substantially conforms with the atomic coordinates represented in Table 3. The conserved amino acids are highlighted in blue in Figure 3a and include G14, G15, G18, H19, G104, H124, E125, G190, G191, S192,

G194, A195, R261, G263, A264, E269, P281, Q289, N292 and A293 (as numbered in the *E. coli* MurG sequence set forth in Figure 3a).

More particularly, a structure that substantially conforms to a given set of atomic coordinates is a structure wherein at least about 50% of such structure has an average root-mean-square deviation (RMSD) of less than about 2.5 A, for the C-alpha backbone and conserved amino acid residue atoms in secondary structure elements in each domain, and more preferably, less than about 2.0 A for the backbone atoms in secondary structure elements in each domain, and, in increasing preference, less than about 1.5 A, less than about 1.0 A, less than about 0.7 A, and more preferably, less than about 0.5 A for the backbone atoms in secondary structure elements in each domain. In a more preferred embodiment, a structure that substantially conforms to a given set of atomic coordinates is a structure wherein at least about 75% of such structure has the recited average rootmean-square deviation (RMSD) value, and more preferably, at least about 90% of such structure has the recited average RMSD value, and most preferably, about 100% of such structure has the recited average RMSD value.

STRUCTURE OF THE DONOR NUCLEOTIDE BINDING SITE OF MurG PROTEINS

An embodiment of the present invention includes the three-dimensional structure of a donor nucleotide binding site of a MurG protein, in particular an *E. coli* MurG protein. A more preferred embodiment of the present invention includes a three-dimensional structure of a donor nucleotide binding site of a MurG protein wherein the three-dimensional structure of the donor nucleotide binding site substantially conforms to the atomic coordinates in Table 4. In a preferred embodiment, the donor nucleotide binding site is a UDP-GlcNAc binding site of a MurG protein.

As described in Example 1, the donor nucleotide binding site is located in the C-terminal domain (see Fig. 4a). This binding site is based on the comparison of β-glucosyltransferase (BGT) and *E. coli* MurG and based on experiments done in our laboratory showing that the isolated C domain binds to a UDP-hexose column (See Example 1). The atomic coordinates of Table 4 set forth the donor nucleotide binding site three-dimensional structure without a donor nucleotide such as UDP-GlcNAc bound to the MurG protein.

According to the present invention, the use of the term "substantially conforms" refers to at least a portion of a three-dimensional structure of a donor nucleotide binding site of a MurG protein which is sufficiently spatially similar to at least a portion of a specified three-dimensional configuration of a particular set of atomic coordinates (e.g., those represented by Table 4) to allow the three-dimensional structure of the donor nucleotide binding domain to be modeled or calculated (i.e., by molecular replacement) using the particular set of atomic coordinates defining the three-dimensional configuration of the donor nucleotide binding site of a MurG protein. According to the present invention, a three-dimensional structure of a given donor nucleotide binding site of a first MurG protein can substantially conform to at least a portion of the atomic coordinates which represent a three-dimensional configuration of a second MurG. Since the atomic coordinates of Table 4 were obtained from the *E. coli* MurG crystal protein without a donor nucleotide bound, there will be some variation from the atomic coordinates of the donor nucleotide binding site when a nucleotide is bound vs. unbound. Therefore, a structure "substantially conforming" to that represented by the atomic coordinates in Table 4, will include a structure obtained from co-crytallization of the protein with a donor nucleotide.

More particularly, a structure that substantially conforms to a given set of atomic coordinates is a structure wherein at least about 50% of such structure has an average root-mean-square deviation (RMSD) of less than about 1.5 Å for the C-alpha backbone atoms in secondary structure elements in each domain, and more preferably, less than about 1.3 Å for the C-alpha backbone atoms in secondary structure elements in each domain, and, in increasing preference, less than about 1.0 Å, less than about 0.7 Å, and more preferably less than about 0.5 Å for the C-alpha backbone atoms in secondary structure elements in each domain. In a more preferred embodiment, a structure that substantially conforms to a given set of atomic coordinates is a structure wherein at least about 75% of such structure has the recited average root-mean-square deviation (RMSD) value, and more preferably, at least about 90% of such structure has the recited average RMSD value.

In an even more preferred embodiment, the above definition of "substantially conforms" can be extended to include atoms of the conserved or invariant amino acid side chains located within the binding site. As used herein, the phrase "conserved

amino acid side chains" refers to amino acid side chains that are conserved between MurG proteins within the donor nucleotide binding site. The conserved amino acid residues of the donor nucleotide binding site have been identified as I125, R261, G263, A264, E269, P281, Q289, N292 and A293 (as numbered in the *E. coli* MurG sequence set forth in Figure 3a) and the G loop found between residues numbered 190-195 having residues G190, G191, S192, G194, and A195. Some or all of these conserved residues are necessary for binding the nucleotide donor.

Preferably, a three-dimensional structure that substantially conforms to a given set of atomic coordinates is a structure wherein at least about 50% of the conserved amino acid side chains have an average RMSD value of less than about 1.5 Å, and more preferably, less than about 1.3 Å, and in increasing preference, less than about 1.0 Å, less than about 0.7 Å, and most preferably, less than about 0.3 Å. In a more preferred embodiment, a structure that substantially conforms to a given set of atomic coordinates is a structure wherein at least about 75% of the conserved amino acid side chains have the recited average RMSD value, and more preferably, at least about 90% of the conserved amino acid side chains have the recited average RMSD value, and most preferably, about 100% of the conserved amino acid side chains have the recited average RMSD value.

STRUCTURE OF THE ACCEPTOR BINDING SITE OF MurG PROTEIN

An embodiment of the present invention includes the three-dimensional structure of an acceptor binding site of a MurG protein. A three-dimensional structure of a acceptor binding site of a MurG protein encompassed by the present invention substantially conforms with the atomic coordinates represented in Table 5. A more preferred embodiment of the present invention includes a three-dimensional structure of an acceptor binding site of a MurG protein wherein the three dimensional structure of the acceptor binding site substantially conforms to the atomic coordinates Table 5.

According to the present invention, the use of the term "acceptors" refers to Lipid I and analogues thereof. For the purposes of obtaining co-crystals containing acceptor analogues bound to the acceptor binding site better, the analogues need not be functional acceptors in a MurG assay. In particular embodiments of the present invention, the acceptor is selected from the group consisting of, but not limited to

Lipid I, and analogs of Lipid I (see compounds described in Ha et al., J. Amer. Chem. Soc. 1999, vol. 121:8415-26, incorporated by herein by reference in its entirety).

As described in Example 1, the acceptor binding site is located in the N-terminal domain of a MurG protein (see Fig. 3a and 4c). The acceptor binding site or domain is characterized by three highly conserved regions, twp of which are glycine-rich loops (also referred to as "G loops") that face the cleft between the C-terminal and N-terminal domains. The conserved residues of the acceptor binding site comprise G14, G15, G18, H19, G104, H124, and E125 (as numbered in the *E. coli* MurG sequence set forth in Figure 3a) and two conserved G loop structures.

According to the present invention, the use of the term "substantially conforms" refers to at least a portion of a three-dimensional structure of an acceptor binding site of a MurG protein which is sufficiently spatially similar to at least a portion of a specified three-dimensional configuration of a particular set of atomic coordinates (e.g., those represented by Table 5) to allow the three-dimensional structure of the acceptor binding site to be modeled or calculated (i.e., by homology modeling) using the particular set of atomic coordinates defining the three-dimensional configuration of the acceptor binding site of a MurG protein. According to the present invention, a three-dimensional structure of a given acceptor binding site of a first MurG protein can substantially conform to at least a portion of the atomic coordinates which represent a three-dimensional configuration of a second MurG.

In an even more preferred embodiment, the above definition of "substantially conforms" can be extended to include atoms of the conserved amino acid side chains. As used herein, the phrase "conserved amino acid side chains" refers to the conserved or invariant amino acid side chains that are common to MurG proteins. Preferably, a three-dimensional structure that substantially conforms to a given set of atomic coordinates is a structure wherein at least about 50% of the conserved amino acid side chains have an average RMSD value of less than about 1.5 Å, and more preferably, less than about 1.3 Å, and in increasing preference, less than about 1.0 Å, less than about 0.7 Å, and most preferably, less than about 0.3 Å. In a more preferred embodiment, a structure that substantially conforms to a given set of atomic coordinates is a structure wherein at least about 75% of the conserved amino acid side chains have the recited average RMSD value, and more preferably, at least about 90% of the conserved amino

acid side chains have the recited average RMSD value, and most preferably, about 100% of the conserved amino acid side chains have the recited average RMSD value.

STRUCTURE OF A MEMBRANE ASSOCIATION SITE OF MurG PROTEIN

An embodiment of the present invention includes the three-dimensional structure of a membrane association site of a MurG protein. A three-dimensional structure of a membrane association site of a MurG protein encompassed by the present invention substantially conforms with the atomic coordinates represented in Table 6. A more preferred embodiment of the present invention includes a three-dimensional structure of an acceptor binding site of a MurG protein wherein the three-dimensional structure of the acceptor binding site substantially conforms to the atomic coordinates in Table 6.

According to the present invention, the use of the term "membrane association site" refers to the region of a MurG protein that associates with cytoplasmic surface of bacterial membranes where it performs the reaction of coupling a soluble donor sugar to the membrane anchored acceptor sugar, Lipid I. Analysis of the *E. coli* MurG protein structure shows a hydrophobic patch consisting of residues 175, L79, F82, W85, and W116 in the N-domain. The membrane association site is where the MurG protein associates with the bacterial membranes, and that it is target for inhibitors if we find that a) we can bind to it with another molecule; b) we can disrupt membrane association by binding to it; or c) disrupting membrane association inhibits activity.

As described in Example 1, the membrane association site is located in the N-terminal domain of a MurG protein (see Fig. 4c). The location of the membrane association site is in close proximity to the acceptor binding site and membrane association in this patch would bring the two M-terminal G-loops close to the membrane surface where the diphosphate portion of the acceptor is located.

According to the present invention, the use of the term "substantially conforms" refers to at least a portion of a three-dimensional structure of a membrane association site of a MurG protein which is sufficiently spatially similar to at least a portion of a specified three-dimensional configuration of a particular set of atomic coordinates (e.g., those represented by Table 6) to allow the three-dimensional structure of the membrane association site to be modeled or calculated (i.e., by molecular replacement) using the particular set of atomic coordinates defining the three-dimensional configuration of the

membrane association site of a MurG protein. According to the present invention, a three-dimensional structure of a given membrane association site of a first MurG protein can substantially conform to at least a portion of the atomic coordinates which represent a three-dimensional configuration of a second MurG.

More particularly, a structure that substantially conforms to a given set of atomic coordinates is a structure wherein at least about 50% of such structure has an average root-mean-square deviation (RMSD) of less than about 1.5 Å for the structural elements in the site, and more preferably, less than about 1.3 Å for the structure elements in each site, and, in increasing preference, less than about 1.0 Å, less than about 0.7 Å, less than about 0.5 Å, and more preferably, less than about 0.3 Å for the structural elements in each site. In a more preferred embodiment, a structure that substantially conforms to a given set of atomic coordinates is a structure wherein at least about 75% of such structure has the recited average root-mean-square deviation (RMSD) value, and more preferably, at least about 90% of such structure has the recited average RMSD value, and most preferably, about 100% of such structure has the recited average RMSD value.

In an even more preferred embodiment, the above definition of "substantially conforms" can be extended to include atoms of α-carbon backbone and conserved amino acid side chains. As used herein, the phrase "conserved amino acid side chains" refers to amino acid side chains that are conserved between MurG proteins. Preferably, a three-dimensional structure that substantially conforms to a given set of atomic coordinates is a structure wherein at least about 50% of the conserved α-carbon backbone and conserved amino acid side chains have an average RMSD value of less than about 1.5 Å, and more preferably, less than about 1.3 Å, and in increasing preference, less than about 1.0 Å, less than about 0.7 Å, and most preferably, less than about. 0.3 Å. In a more preferred embodiment, a structure that substantially conforms to a given set of atomic coordinates is a structure wherein at least about 75% of the α-carbon backbone and conserved amino acid side chains have the recited average RMSD value, and more preferably, at least about 90% of the α-carbon backbone and conserved acid side chains have the recited average RMSD value, and most preferably, about 100% of the α-carbon and conserved amino acid side chains have the recited average RMSD value.

COMPUTER READABLE MEDIUM

Another embodiment of the present invention relates to a computer-readable medium encoded with a set three-dimensional coordinates seleceted from the group consisting of the three-dimensional coordinates represented in Table l, the three-dimensional coordinates represented in Table 2, the three-dimensional coordinates represented in Table 3, the three-dimensional coordinates represented in Table 4, the three-dimensional coordinates represented in Table 5, or the three-dimensional coordinates represented in Table 6, wherein using a graphical display software program, the three-dimensional coordinates create an electronic file that can be visualized on a computer capable of representing said electronic file as a three-dimensional image. Preferably, the three-dimensional image is of a MurG protein, the α-carbon backbone of MurG, the α-carbon backbone and conserved amino acid residue sidechains of MurG, the donor nucleotide binding site of MurG, the acceptor binding site of MurG, or the membrane association site of MurG.

Yet another embodiment of the present invention relates to a computer-readable medium encoded with a set of three-dimensional coordinates of a three-dimensional structure which substantially conforms to the three-dimensional coordinates represented in Table 1, wherein using a graphical display software program, the three-dimensional coordinates create an electronic file that can be visualized on a computer capable of representing said electronic file as a three-dimensional image. In other embodiments, the present invention relates to a computer-readable medium encoded with a set of three-dimensional coordinates of a three-dimensional structure which substantially conforms to the three-dimensional coordinates represented in Table 2, Table 3, Table 4, Table 5 or Table 6, wherein using a graphical display software program, the three-dimensional coordinates create an electronic file that can be visualized on a computer capable of representing said electronic file as a three-dimensional image. Preferably, the three-dimensional image is of a MurG protein, the α-carbon backbone of MurG, the α-carbon backbone and conserved amino acid residue sidechains of MurG, the donor nucleotide binding site of MurG, the acceptor binding site of MurG, or the membrane association site of MurG.

IMAGES

One embodiment of the present invention relates to a two dimensional image of an *E. coli* MurG protein including those illustrated in Figures 3-4. Most of these figures were drawn with the MOLSCRIPT program. Preferably, the two dimensional image is of a MurG protein, the α-carbon backbone of MurG, the α-carbon backbone and conserved amino acid residue sidechains of MurG, the donor nucleotide binding site of MurG, the acceptor binding site of MurG, or the membrane association site of MurG.

Another embodiment of the present invention includes a three-dimensional computer image of the three-dimensional structure of a MurG protein, preferably the *E. coli* MurG protein. Suitable structures of which to produce three-dimensional computer images are disclosed herein. Preferably, a computer image is created to a structure substantially conforming with the three-dimensional coordinates represented in Table 1.

Another embodiment of the present invention includes an image of an MurG protein that is generated when a set of three-dimensional coordinates comprising the three-dimensional coordinates represented in Table 1 are analyzed on a computer using a graphical display software program to create an electronic file of the image and visualizing the electronic file as a three-dimensional image. Suitable structures to image are disclosed herein. Preferably, the three-dimensional structures are of a MurG protein, the α-carbon backbone of MurG, the α-carbon backbone and conserved amino acid residue sidechains of MurG, the donor nucleotide binding site of MurG, the acceptor binding site of MurG, or the membrane association site of MurG. Most preferably, the MurG protein is the *E. coli* MurG protein described herein. A computer image of the present invention can. be produced using any suitable software program, including, but not limited to, MOLSCRIPT 2.0 (Avatar Software AB, Helenebrgsgatan 21 C, SE-11713, Stockholm, Sweden), the graphical display program O (Jones et al., Acta Crystallography, vol. A47, p. 110, 1991), or the graphical display program GRASP. Suitable computer hardware useful for producing an image of the present invention are known to those of skill in the art. Preferred computer hardware includes a Silicon Graphics Workstation.

MODELS OF MurG PROTEINS AND BINDING SITES

According to the present invention, a three-dimensional structure of the *E. coli* MurG protein and its binding sites of the present invention can be used to derive a model of the three-dimensional structure of another MurG protein and its binding sites (i.e., a structure to be modeled). As used herein, a "structure" of a protein refers to the components and the manner of arrangement of the components to constitute a protein or binding site. Also, as used herein, the term "model" refers to a representation of a tangible medium of the three-dimensional structure of a protein, polypeptide or peptide, or binding site of a protein. For example, a model can be a representation of the three-dimensional structure in a electronic file, on a computer screen, on a piece of paper (i.e., on a two dimensional medium), and/or as a ball-and-stick figure. Physical three-dimensional models are tangible and include, but are not limited to, stick models and space-filling models. The phrase "imaging the model on a computer screen" refers to the ability to express (or represent) and manipulate the model on a computer screen using appropriate computer hardware and software technology known to those skilled in the art. Such technology is available from a variety of sources including, for example, Evans and Sutherland, Salt Lake City, Utah, and Biosym Technologies, San Diego, CA. The phrase "providing a picture of the model" refers to the ability to generate a "hard copy" of the model. Computer screen images and pictures of the model can be visualized in a number of formats including space-filling representations, α-carbon traces, ribbon diagrams and electron density maps.

Suitable target MurG proteins and their associated binding sites to model using a method of the present invention include any MurG protein and binding sites that are at least in part structurally related to the *E. coli* MurG protein or its binding sites. A preferred target MurG structure that is at least in part structurally related includes a target MurG structure having an amino acid sequence that is at least about 25%, preferably at least about 30%, more preferably at least about 36%, more preferably at least about 40%, even more preferably at least about 50%, more preferably at least about 60%, more preferably at least about 70%, more preferably at least about 80%, and more preferably at least about 90% identical to an amino acid sequence of the *E. coli* MurG protein, across the full-length of the target MurG structure sequence when using, for example, a sequence alignment program such as DNAsis™ program (available from

Hitachi Software, San Bruno, CA) or the MacVector™ program (available from the Eastman Kodak Company, New Haven, CT) or the GCγ™ program (available from the "GCγ", University of Wisconsin, Madison, WI), such alignment being performed for example, using the standard default values accompanying such alignment programs.

Preferred MurG proteins and their binding sites are set forth in the amino acid sequences of MurG proteins as deposited in the NCBI database and are identified with Accession Nos. CAB51993, A71316, E70579, C71699, F70195, A43727, JC1275, BVECMG, CEECAM, 083535, Q9ZK59, CAB85280, AAF39020, BAA18775, AAD26629, CAB73295, P37585, Q9ZHA9, Q9ZHDC0, Q9ZBA5, Q9X4H4, Q9WY74, P74657, O06224, Q9Z702, O84766, O69552, O67238, O51708, O25770, O07670, O07109, P45065, CAB66324, AAC68356, AAF06830, P18579, P17443, P17952, P16457, P07862, AAE23178, AAD53936, CAA18668, CAA38869, CAA38868, CAA38867, CAA38866, AAD08196, BAA01453, BAA01455, BAA01454, AAD19042, CAA45558, CAA74235, AAD10537, AAD06652, AAC95450, CAA14869, AAC73201, AAC65509, AAC67113, AAC45636, CABO8640, AAC22793, AAC07193, BAA24357, CAB13395, BAA01355, AAB35538, 1904153C, 1808265B, 1808265A, CAA36866, CAA36869, CAA36868, CAA36867, CAA36776, and AAA99436. The amino acid sequences are publicly available.

A variety of MurG proteins from numerous organisms can be used to prepare models of MurG proteins and binding sites, including but not limited to, microorganisms such as bacteria, higher-order bacteria, thermal stable bacteria, spirochetes, small pathogenic organisms, fungi, protozoa, cyanobacteria, and trypanosomes. More particularly, bacteria such as but not limited to, *Escherichia coli, Bacillus subtilis, Aquefex aeolicus, Borrelia burgdorferi, Chlamydia pneumoniae, Chlamydia trachomatis, Enterococcus faecais, Enterococcus hirae, Haemophilus influenzae, Helicobacter pyloir J99 , Helicobacter pylori, Mycobacterium tuberculosis, Porphyromonas gingivalis, Rickettsia prowazekii, Streptomyces coelicolor, Streptomyces collinus, Streptococcus pneumoniae, Synechocystis* sp. (strain PCC6803), *Thermotoga maritime,* and *Treponema pallidum.* It is noted that nucleotide and amino acid sequences for many of the above identified organisms are known and publicly available.

Preferred target MurG proteins and binding site structures to model also include, but are not limited to, derivatives of MurG proteins, such as a MurG protein having one or more amino acid residues substituted, deleted or added (referred to herein as MurG mutants), or proteins encoded by natural variants of a nucleic acid molecule encoding a MurG.

In another embodiment of the invention, the process of building a homology model for a protein is divided into the following steps:

(1) Determine which proteins are related to the model protein;

(2) Determine structurally conserved regions (SCRs);

(3) Align the amino acid sequence of the unknown protein with those of the reference protein(s) within the SCRs;

(4) Assign coordinates in the conserved regions;

(5) Predict conformations for the rest of the peptide chain, including loops between the SCRs and possibly the N- and C-termini;

(6) Search for the optimum side chain conformations for residues that differ from those in the reference proteins; and

(7) Use energy minimization and molecular dynamics to refine the molecular structure so that steric strain introduced during the model-building process can be relieved.

Published sequences are readily available through on-line databases on the Internet, such as SwissProt (http://www.expasy.ch/sprot/sprot-top.html). MurG specific and related sequences are obtained for use for building homology models by text-based or sequence similarity searching. SCRs for MurG is the entire protein, considering the *E. coli* MurG crystal structure is the only similar sequence with structural data. Alignment of the sequences using an appropriate alignment program and algorithm, such as Clustal W, allows appropriate assignment of the *E. coli* protein coordinates to a MurG sequence of unknown structure. The Modeler program performs the conformational predictions for the peptide chain and side chains. Dynamics and minimization using an appropriate program and algorithm, such as Discover.

Modeler Description:

Modeler is an automated homology-modeling scheme designed to find the most probable three-dimensional structure of a protein, given its amino acid sequence and its

alignment with related structures. It derives 3D protein models without the time consuming separate stages of core region identification and loop region building or searching that is inherent to manual homology modeling schemes. The related or reference protein structures are used to derive spatial restraints expressed as probability density functions (PDFs) for each of the restrained features of the model. As an example, the main chain conformation of a given residue in the model will be described by restraints that depend upon the residue type, the main chain conformation of equivalent residues in the reference proteins and the local sequence similarity. The probability distribution functions that are used in restraining the model structure are derived from correlations between structural features in a database of families of homologous proteins aligned on the basis of their 3D structure. These functions are used to restrain C-C distances, main chain N--O distances, main chain and side chain dihedral angles, etc. The individual restraints are assembled into a single molecular probability density function (MPDF). The three-dimensional protein model is then obtained by an optimization of this MPDF. The optimization procedure itself consists of a variable target function method (Braun and Go, 1985) with conjugate gradient minimization scheme followed by an optional restrained simulated annealing molecular dynamics scheme.

While several reference structures are used in the traditional homology model building process, only one set of coordinates can be used in any one peptide segment. Modeler is able to simultaneously incorporate structural data from one or more reference proteins. Structural features in the reference proteins are used to derive spatial restraints which in turn are used to generate model protein structures using conjugate gradient and simulated annealing optimization procedures.

Clustal W description:

Clustal W aligns multiple sequences using a progressive pairwise alignment algorithm. It first generates all possible pairwise alignments for a list of sequences and then builds the guide tree based on their pairwise sequence identity, aligning the sequences following the order of the guide tree.

Several unique features in Clustal W improve the sensitivity of the alignment of divergent protein sequences (Thompson et al, 1994a).

(1) Individual weights are assigned to each sequence in a partial alignment in order to downweight near-duplicate sequences and upweight the most divergent ones.

(2) Amino acid substitution matrices are varied at different alignment stages according to the divergence of the sequences to be aligned.

(3) Residue-specific gap penalties and locally reduced gap penalties in hydrophilic regions encourage new gaps in potential loop regions rather than regular secondary structure.

(4) Positions in early alignments, where gaps have been opened, receive locally reduced gap penalties to encourage the opening of new gaps at these positions.

Discover Description:

The Discover program performs energy minimization, template forcing, torsion forcing, and dynamic trajectories and calculates properties such as interaction energies, derivatives, mean square displacements, and vibrational frequencies. It provides tools for performing simulations under various conditions including constant temperature, constant pressure, constant stress, periodic boundaries, and fixed and restrained atoms.

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STRUCTURE BASED DRUG DESIGN

The present invention relates to the use of the crystal structure of the *E. coli* MurG protein represented by the atomic coordinates in Table 1 to make models of MurG proteins and binding sites thereof. The present invention also relates to the use of the crystal structure, α-carbon backbone, α-carbon backbone plus conserved amino acid residue side chains or binding sites of the *E. coli* MurG protein to construct models of these structures in other MurG proteins.

For the first time, the present invention permits the use of molecular design techniques to design, select and synthesize chemical entities and compounds, including inhibitory compounds, capable of binding to the active site or accessory binding site of MurG, in whole or in part.

On approach enabled by this invention, is to use the structure coordinates of MurG to design compounds that bind to the enzyme and alter the physical properties of the compounds in different ways, e.g., solubility. For example, this invention enables the design of compounds that act as inhibitors of the MurG enzyme by binding to, all or a portion of, the active site of MurG.

A second design approach is to probe a MurG crystal with molecules composed of a variety of different chemical entities to determine optimal sites for interaction between candidate MurG inhibitors and the enzyme. For example, high resolution X-ray diffraction data collected from crystals saturated with solvent allows the determination of where each type of solvent molecule sticks. Small molecules that bind

tightly to those sites can then be designed and synthesized and tested for their MurG inhibitor activity. Travis, J., Science, 262, p. 1374 (1993).

This invention also enables the development of compounds that can isomerize to short-lived reaction intermediates in the chemical reaction of a substrate or other compound that binds to MurG, with MurG. Thus, the time-dependent analysis of structural changes in MurG during its interaction with other molecules is enabled. The reaction intermediates of MurG can also be deduced from the reaction product in co-complex with MurG. Such information is useful to design improved analogues of known MurG inhibitors or to design novel classes of inhibitors based on the reaction intermediates of the MurG enzyme and MurG-inhibitor co-complex. This provides a novel route for designing MurG inhibitors with both high specificity and stability.

Another approach made possible and enabled by this invention, is to screen computationally small molecule data bases for chemical entities or compounds that can bind in whole, or in part, to the MurG enzyme. In this screening, the quality of fit of such entities or compounds to the binding site may be judged either by shape complementarity or by estimated interaction energy. Meng, E. C. et al., J. Coma. Chem., 13, pp.505-524 (1992).

Because MurG may crystallize in more than one crystal form, the structure coordinates of MurG, or portions thereof, as provided by this invention are particularly useful to solve the structure of those other crystal forms of MurG. They may also be used to solve the structure of MurG mutants, MurG co-complexes, or of the crystalline form of any other protein with significant amino acid sequence homology to any functional domain of MurG.

One method that may be employed for this purpose is molecular replacement. In this method, the unknown crystal structure, whether it is another crystal form of MurG a MurG mutant, or a MurG co-complex, or the crystal of some other protein with significant amino acid sequence homology to any functional domain of MurG, may be determined using the MurG structure coordinates of this invention as provided in Tables 1-6. This method will provide an accurate structural form for the unknown crystal more quickly and efficiently than attempting to determine such information ab initio.

In addition, in accordance with this invention, MurG mutants may be crystallized in co-complex with known MurG inhibitors. The crystal structures of a series of such complexes may then be solved by molecular replacement and compared with that of wild-type MurG. Potential sites for modification within the various binding sites of the enzyme may thus be identified. This information/provides an additional tool for determining the most efficient binding interactions, for example, increased hydrophobic interactions, between MurG and a chemical entity or compound.

All of the complexes referred to above may be studied using well-known X-ray diffraction techniques and may be refined versus 2-3 .ANG. resolution X-ray date to an R value of about 0.20 or less using computer software, such as X-PLOR (Yale University, .COPYRGT.1992, distributed by Molecular Simulations, Inc.). See, e.g., Blundel & Johnson, supra; Methods in Enzvmoloav, vol. 114 & 115, H. W. Wyckoff et al., eds., Academic Press (1985). This information may thus be used to design, synthezie and optimize novel classes of MurG inhibitors.

The structure coordinates of MurG mutants provided in this invention also facilitate the identification of related proteins or enzymes analogous to MurG in function, structure or both, thereby further leading to novel therapeutic modes for treating or preventing UDP-glycosyltransferase mediated diseases.

The design of compounds that bind to or inhibit MurG according to this invention generally involves consideration of two factors. First, the compound must be capable of physically and structurally associating with MurG. Non-covalent molecular interactions important in the association of MurG with its substrate include hydrogen bonding, van der Waals and hydrophobic interactions.

Second, the compound must be able to assume a conformation that allows it to associate with MurG. Although certain portions of the compound will not directly participate in this association with MurG, those portions may still influence the overall conformation of the molecule. This, in turn, may have a significant impact on potency. Such conformational requirements include the overall three-dimensional structure and orientation of the chemical entity or compound in relation to all or a portion of the binding site, e.g., active site or accessory binding site of MurG, or the spacing between functional groups of a compound comprising several chemical entities that directly interact with MurG.

The potential inhibitory or binding effect of a chemical compound on MurG may be analyzed prior to its actual synthesis and testing by the use of computer modelling techniques. If the theoretical structure of the given compound suggests insufficient interaction and association between it and MurG, synthesis and testing of the compound is obviated. However, if computer modelling indicates a strong interaction, the molecule may then be synthesized and tested for its ability to bind to MurG and inhibit using the assay of Walker et al. patents (cited supra). In this manner, synthesis of inoperative compounds may be avoided.

An inhibitory or other binding compound of MurG may be computationally evaluated and designed by means of a series of steps in which chemical entities or fragments are screened and selected for their ability to associate with the individual binding pockets or other areas of MurG.

One skilled in the art may use one of several methods to screen chemical entities or fragments for their ability to associate with MurG and more particularly with the individual binding pockets of the MurG donor nucleotide binding site, acceptor binding site or membrane association site. This process may begin by visual inspection of, for example, the binding sites on the computer screen based on the MurG coordinates in Tables 1-6. Selected fragments or chemical entities may then be positioned in a variety of orientations, or docked, within an individual binding pocket of MurG as defined supra. Docking may be accomplished using software such as Quanta and Sybyl, followed by energy minimization and molecular dynamics with standard molecular mechanics forcefields, such as CHARMM and AMBER.

Specialized computer programs may also assist in the process of selecting fragments or chemical entities, including but not limited to:

1. GRID (Goodford, P. J., "A Computational Procedure for Determining Energetically Favorable Binding Sites on Biologically Important Macromolecules" J. Med. Chem., 28, pp.849-857 (1985)). GRID is available &orn Oxford University, Oxford, UK.

2. MCSS (Miranker, A. and M. Karplus, "Functionality Maps of Binding Sites: A Multiple Copy Simultaneous Search Method." Proteins: Structure, Function and Genetics, 11, pp.29-34 (1991)). MCSS is available from Molecular Simulations, Burlington, Mass.

3. AUTODOCK (Goodsell, D. S. and A. J. Olsen, "Automated Docking of Substrates to Proteins by Simulated Annealing" Proteins: Structure. Function, and Genetics, 8, pp.195-202 (1990)) (AUTODOCK is available from Scripps Research Institute, La Jolla, Calif.).

4. DOCK (Kuntz, 1. D. et al., "A Geometric Approach to Macromolecule-Ligand Interactions" J. Mol. Biol., 161, pp.269-288 (1982)). DOCK is available from University of California, San Francisco, Calif.

Once suitable chemical entities or fragments have been selected, they can be assembled into a single compound or inhibitor. Assembly may be proceeded by visual inspection of the relationship of the fragments to each other on the three-dimensional image displayed on a computer screen in relation to the structure coordinates of MurG. This would be followed by manual model building using software such as Quanta or Sybyl.

Useful programs to aid one of skill in the art in connecting the individual chemical entities or fragments include, but are not limited to:

1. CAVEAT (Bartlett, P. A. et al, "CAVEAT: A Program to Facilitate the Structure-Derived Design of Biologically Active Molecules". In Molecular Recognition in Chemical and Biological Problems", Special Pub., Royal Chem. Soc., 78, pp.182-196 (1989)). CAVEAT is available from the University of California, Berkeley, Calif.

2. 3D Database systems such as MACCS-3D (MDL Information Systems, San Leandro, Calif). This area is reviewed in Martin, Y. C., "3D Database Searching in Drug Design", J. Med. Chem., 35, pp.2145-2154 (1992)).

3. HOOK (available from Molecular Simulations, Burlington, Mass.).

Instead of proceeding to build a MurG inhibitor in a step-wise fashion one fragment or chemical entity at a time as described above, inhibitory or other MurG binding compounds may be designed as a whole or "de novo" using either an empty active site or optionally including some portion(s) of a known inhibitor(s). These methods include, but are not limited to:

1. LUDI (Bohm, H.-J., "The Computer Program LUDI: A New Method for the De Novo Design of Enzyme Inhibitors", J. ComR. Aid. Molec. Design, 6, pp.61-78 (1992)). LUDI is available from Biosym Technologies, San Diego, Calif.

2. LEGEND (Nishibata, Y. and A. Itai, Tetrahedron, 47, p. 8985 (1991)). LEGEND is available from Molecular Simulations, Burlington, Mass.

3. LeapFrog (available from Tripos Associates, St. Louis, Mo.).

Other molecular modeling techniques may also be employed in accordance with this invention. See, e.g., Cohen, N. C. et al., "Molecular Modeling Software and Methods for Medicinal Chemistry", J. Med. Chem., 33, pp.883-894 (1990). See also, Navia, M. A. and M. A. Murcko, "The Use of Structural Information in Drug Design", Current Opinions in Structural Biology, 2, pp. 202-210 (1992).

Once a compound has been designed or selected by the above methods, the efficiency with which that compound may bind to MurG may be tested and optimized by computational evaluation. For example, a compound that has been designed or selected to function as a MurG-inhibitor must also preferably traverse a volume not overlapping that occupied by the active site when it is bound to the native substrate. An effective MurG inhibitor must preferably demonstrate a relatively small difference in energy between its bound and free states (i.e., a small deformation energy of binding). Thus, the most efficient MurG inhibitors should preferably be designed with a deformation energy of binding of not greater than about 10 kcal/mole, preferably, not greater than 7 kcal/mole. MurG inhibitors may interact with the enzyme in more than one conformation that is similar in overall binding energy. In those cases, the deformation energy of binding is taken to be the difference between the energy of the free compound and the average energy of the conformations observed when the inhibitor binds to the enzyme.

A compound designed or selected as binding to MurG may be further computationally optimized so that in its bound state it would preferably lack repulsive electrostatic interaction with the target enzyme. Such non-complementary (e.g., electrostatic) interactions include repulsive charge-charge, dipole-dipole and charge-dipole interactions. Specifically, the sum of all electrostatic interactions between the inhibitor and the enzyme when the inhibitor is bound to MurG, preferably make a neutral or favorable contribution to the enthalpy of binding.

Specific computer software is available in the art to evaluate compound deformation energy and electrostatic interaction. Examples of programs designed for such uses include, but are not limited to: Gaussian 92, revision C [M. J. Frisch,

Gaussian, Inc., Pittsburgh, Pa. COPYRIGHT. 1992]; AMBER, version 4.0 [P. A. Kollman, University of California at San Francisco, COPYRIGHT. 1994]; QUANTA/CHARMM [Molecular Simulations, Inc., Burlington, Mass. COPYRIGHT. 1994]; and Insight II/Discover (Biosysm Technologies Inc., San Diego, Calif COPYRIGHT. 1994). These programs may be implemented, for instance, using a Silicon Graphics workstation, IRIS Octane or IBM RISC/6000 workstation. Other hardware systems and software packages will be known to those skilled in the art.

Once a MurG-binding compound has been optimally selected or designed, as described above, substitutions may then be made in some of its atoms or side groups in order to improve or modify its binding properties. Generally, initial substitutions are conservative, i.e., the replacement group will have approximately the same size, shape, hydrophobicity and charge as the original group. It should, of course, be understood that components known in the art to alter conformation should be avoided. Such substituted chemical compounds may then be analyzed for efficiency of fit to MurG by the same computer methods described in detail, above.

COMPOUNDS AND COMPOSITIONS COMPRISING COMPOUNDS DERIVED FROM STRUCTURE BASED DRUG DESIGN

One embodiment of the present invention is a compound that is capable of binding to a MurG protein, inhibiting the activity of a MurG protein, or stimulating the activity of a MurG protein. Suitable inhibitory compounds of the present invention can: (1) inhibit (i.e., prevent or block) the activity of MurG enzyme by binding to a MurG donor nucleotide binding site and interfering with the binding of the donor nucleotide molecule; (2) inhibit the activity of MurG enzyme by binding to the MurG acceptor binding site and interfering with the binding of the acceptor molecule; (3) inhibit the activity of a MurG enzyme by binding to the membrane association site and interfering with the association of the protein with the bacterial membrane and/or acceptor molecule.

Another embodiment of the present invention is a compound that is capable of stimulating MurG activity. Suitable stimulatory compounds of the present invention can stimulate the activity of a MurG enzyme by binding to the protein at a binding site and causing an increase in enzymatic activity, for example, by increasing the enzymes

affinity to bind a donor nucleotide, an acceptor molecule or improve the enzymes stability or increasing the binding affinity of a molecule to MurG.

Such compounds that bind to, inhibit or stimulate activity of a MurG protein include, for example, compounds that mimic donor nucleotide molecules. In preferred embodiments, the compound includes, for example, pyrimidine nucleoside analogues. In yet another preferred embodiment, the compounds include compounds comprising a pyrimidine nucleoside with a substituent containing at least one heteroatom attached to the C5 hydroxyl. In more particular embodiments, pyrimidine derivatives make complementary hydrogen bonding contacts to the amide backbone segment containing Ile 245 and also contact glutamate 269.

Another embodiment of the present invention is a compound that binds to the acceptor binding site of the MurG protein, hereinafter referred to a acceptor analogs. An acceptor analog refers to a compound that interacts with (e.g., binds to, associates with, modifies) the acceptor binding site of a MurG protein. An acceptor analog, for example, is a compound that mimics the natural acceptor molecule, Lipid I. Examples of such acceptor analogs are set forth in Ha et al., J. Amer. Chem. Soc. 1999, and PCT/US99/02187, U.S. Provisional Application No. 60/073,376 filed February 2, 1998, incorporated herein by reference.

Another embodiment of the present invention is a compound that binds to the MurG protein, that are enzyme product analogs, hereinafter referred to as Lipid II analogs. A Lipid II analog refers to a compound that interacts with (i.e., binds to, associates with, modifies) the acceptor binding site of a Mur G protein which mimics the product of the transglycosylase reaction.

Inhibitory and stimulatory compounds of the present invention can be identified by various means known to those of skill in the art. For example, binding of an inhibitory compound to, or otherwise interaction with, a MurG protein, can be determined with MurG in solution, for example, using assays described in PCT/US99/02187, U.S. Provisional Application No. 60/073,376 filed February 2, 1998, and PCT/US00/05554 , U.S. Provisional Application Nos. 60/122,966 and 60/137,696, incorporated herein by reference.

According to the present invention, suitable compounds of the present invention include peptides or other organic molecules, and inorganic molecules. Suitable organic

molecules include small organic molecules. Preferably, a compound of the present invention is not harmful (i.e., toxic) to an animal when administered to an animal.

Compounds of the present invention also can be identified using structure based drug design techniques known to those skilled in the art and described herein above.

Also according to the present invention, compounds are suitable for use in the inhibition of bacterial or microbial growth in an animal, and for example, function as an antibiotic for treatment of bacterial infections in animals.

The present invention also includes compositions comprising compounds of the present invention that inhibit or stimulate MurG activity which function as antibiotics or antimicrobial agents in animals. Compositions of the present invention can be used therapeutically or diagnostically in an animal. Compositions of the present invention comprises at least one compound of the present invention. In a preferred embodiment, compositions of the present invention further comprise a carrier. More particularly, a suitable carrier is a pharmaceutically acceptable carrier known to those skilled in the art.

TABLE 1- ATOMIC COORDINATES OF E. COLI MURG PROTEIN

REMARK coordinates from minimization refinementREMARK refinement resolution: 40.0 - 1.9 AREMARK starting r= 0.2200 free_r= 0.2466REMARK final r= 0.2200 free_r= 0.2466REMARK rmsd bonds= 0.005558 rmsd angles= 1.29505REMARK wa= 1.08391REMARK target= mlf cycles= 1 steps= 30REMARK sg= P1 a= 60.613 b= 66.356 c= 67.902 alpha= 64.294 beta= 83.520 gamma= 65.448REMARK parameter file 1 :
CNS_TOPPAR:protein_rep.paramREMARK parameter file 2 :
CNS_TOPPAR:water_rep.paramREMARK parameter file 3 :
CNS_TOPPAR:ion.paramREMARK molecular structure file: gen.mtfREMARK input coordinates: gen.pdbREMARK reflection file= native.cvREMARK ncs= noneREMARK B-correction resolution: 6.0 - 1.9REMARK initial B-factor correction applied to fobs :REMARK B11= 0.747 B22= 2.098 B33= -2.845REMARK B12= -1.847 B13= -3.752 B23= 6.401REMARK B-factor correction applied to coordinate array B: 0.038REMARK bulk solvent: density level= 0.351665 e/A^3, B-factor= 43.8282 A^2REMARK reflections with |Fobs|/sigma_F < 2.0 rejectedREMARK reflections with |Fobs| > 10000 * rms(Fobs) rejectedREMARK theoretical total number of refl. in resol. range:68102 (100.0%)REMARK number of unobserved reflections (no entry or |F|=0):2825(4.1%) REMARK number of reflections rejected:
3288 (4.8 %)REMARK total number of reflections used:
61989 91.0%)REMARK number of reflections in working set:
55765 (81.9%)REMARK number of reflections in test set:
6224 (9.1%)CRYST1 60.613 66.356 67.902 64.29 83.52 65.45 P 1
REMARK FILENAME="minimize5.pdb"REMARK DATE:14-Jan-00 15:25:36
created by user: shaREMARK VERSION:
0.5

ATOM	1	CB	LYS	A	7	0.142	3.434	35.023	1.00	43.02 AAAA
ATOM	2	CG	LYS	A	7	1.076	4.457	35.641	1.00	46.34 AAAA
ATOM	3	CD	LYS	A	7	0.452	5.841	35.634	1.00	47.39 AAAA
ATOM	4	CE	LYS	A	7	1.345	6.846	36.332	1.00	48.65 AAAA
ATOM	5	NZ	LYS	A	7	0.780	8.221	36.276	1.00	51.04 AAAA
ATOM	6	C	LYS	A	7	-2.239	2.733	34.833	1.00	39.64 AAAA
ATOM	7	O	LYS	A	7	-2.050	1.717	34.160	1.00	39.64 AAAA
ATOM	8	N	LYS	A	7	-0.974	2.320	36.947	1.00	42.05 AAAA
ATOM	9	CA	LYS	A	7	-1.170	3.245	35.788	1.00	41.31 AAAA
ATOM	10	N	ARG	A	8	-3.357	3.451	34.773	1.00	37.24 AAAA
ATOM	11	CA	ARG	A	8	-4.469	3.076	33.906	1.00	34.91 AAAA
ATOM	12	CB	ARG	A	8	-5.782	3.109	34.686	1.00	36.65 AAAA
ATOM	13	CG	ARG	A	8	-5.950	2.017	35.721	1.00	39.89 AAAA
ATOM	14	CD	ARG	A	8	-7.323	2.124	36.356	1.00	42.12 AAAA
ATOM	15	NE	ARG	A	8	-7.663	0.960	37.163	1.00	45.03 AAAA
ATOM	16	CZ	ARG	A	8	-7.031	0.610	38.279	1.00	46.29 AAAA
ATOM	17	NH1	ARG	A	8	-6.015	1.337	38.725	1.00	46.88 AAAA
ATOM	18	NH2	ARG	A	8	-7.420	-0.466	38.952	1.00	47.41 AAAA
ATOM	19	C	ARG	A	8	-4.584	3.999	32.696	1.00	32.27 AAAA
ATOM	20	O	ARG	A	8	-4.602	5.224	32.832	1.00	31.60 AAAA
ATOM	21	N	LEU	A	9	-4.663	3.403	31.512	1.00	29.57 AAAA
ATOM	22	CA	LEU	A	9	-4.792	4.171	30.283	1.00	27.45 AAAA
ATOM	23	CB	LEU	A	9	-3.581	3.954	29.362	1.00	26.31 AAAA
ATOM	24	CG	LEU	A	9	-3.752	4.466	27.916	1.00	25.77 AAAA
ATOM	25	CD1	LEU	A	9	-3.670	5.985	27.895	1.00	24.31 AAAA

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ATOM     26  CD2 LEU A   9      -2.679   3.870  26.993  1.00 26.22 AAAA
ATOM     27  C   LEU A   9      -6.038   3.762  29.523  1.00 25.97 AAAA
ATOM     28  O   LEU A   9      -6.397   2.587  29.485  1.00 25.57 AAAA
ATOM     29  N   MET A  10      -6.713   4.738  28.928  1.00 25.37 AAAA
ATOM     30  CA  MET A  10      -7.866   4.429  28.101  1.00 24.70 AAAA
ATOM     31  CB  MET A  10      -9.142   5.101  28.612  1.00 25.60 AAAA
ATOM     32  CG  MET A  10     -10.323   4.873  27.675  1.00 25.77 AAAA
ATOM     33  SD  MET A  10     -11.916   4.958  28.492  1.00 26.63 AAAA
ATOM     34  CE  MET A  10     -12.197   3.222  28.862  1.00 25.72 AAAA
ATOM     35  C   MET A  10      -7.528   4.943  26.715  1.00 23.31 AAAA
ATOM     36  O   MET A  10      -7.198   6.116  26.544  1.00 24.02 AAAA
ATOM     37  N   VAL A  11      -7.574   4.059  25.727  1.00 22.25 AAAA
ATOM     38  CA  VAL A  11      -7.278   4.461  24.359  1.00 22.34 AAAA
ATOM     39  CB  VAL A  11      -6.444   3.386  23.624  1.00 22.75 AAAA
ATOM     40  CG1 VAL A  11      -6.256   3.768  22.158  1.00 20.51 AAAA
ATOM     41  CG2 VAL A  11      -5.082   3.239  24.310  1.00 21.75 AAAA
ATOM     42  C   VAL A  11      -8.612   4.654  23.646  1.00 22.94 AAAA
ATOM     43  O   VAL A  11      -9.525   3.843  23.804  1.00 23.37 AAAA
ATOM     44  N   MET A  12      -8.722   5.734  22.878  1.00 22.18 AAAA
ATOM     45  CA  MET A  12      -9.949   6.034  22.146  1.00 23.10 AAAA
ATOM     46  CB  MET A  12     -10.496   7.399  22.589  1.00 22.78 AAAA
ATOM     47  CG  MET A  12     -10.359   7.655  24.096  1.00 23.92 AAAA
ATOM     48  SD  MET A  12     -10.955   9.279  24.657  1.00 25.51 AAAA
ATOM     49  CE  MET A  12      -9.641  10.349  24.162  1.00 22.79 AAAA
ATOM     50  C   MET A  12      -9.582   6.072  20.673  1.00 22.97 AAAA
ATOM     51  O   MET A  12      -8.917   6.997  20.226  1.00 21.16 AAAA
ATOM     52  N   ALA A  13      -9.992   5.057  19.921  1.00 26.97 AAAA
ATOM     53  CA  ALA A  13      -9.665   5.008  18.498  1.00 30.88 AAAA
ATOM     54  CB  ALA A  13      -8.381   4.212  18.288  1.00 31.18 AAAA
ATOM     55  C   ALA A  13     -10.813   4.412  17.685  1.00 34.35 AAAA
ATOM     56  O   ALA A  13     -11.328   3.335  18.006  1.00 35.86 AAAA
ATOM     57  N   GLY A  14     -11.176   5.127  16.622  1.00 37.37 AAAA
ATOM     58  CA  GLY A  14     -12.287   4.762  15.757  1.00 40.54 AAAA
ATOM     59  C   GLY A  14     -12.239   3.583  14.808  1.00 41.52 AAAA
ATOM     60  O   GLY A  14     -11.267   2.831  14.755  1.00 43.26 AAAA
ATOM     61  N   GLY A  15     -13.322   3.451  14.042  1.00 42.70 AAAA
ATOM     62  CA  GLY A  15     -13.491   2.363  13.094  1.00 43.13 AAAA
ATOM     63  C   GLY A  15     -12.660   2.286  11.825  1.00 43.41 AAAA
ATOM     64  O   GLY A  15     -13.212   2.187  10.730  1.00 44.39 AAAA
ATOM     65  N   THR A  16     -11.340   2.333  11.966  1.00 43.38 AAAA
ATOM     66  CA  THR A  16     -10.426   2.204  10.833  1.00 43.22 AAAA
ATOM     67  CB  THR A  16     -10.120   3.551  10.110  1.00 44.23 AAAA
ATOM     68  OG1 THR A  16      -9.302   4.375  10.949  1.00 44.41 AAAA
ATOM     69  CG2 THR A  16     -11.404   4.286   9.754  1.00 43.74 AAAA
ATOM     70  C   THR A  16      -9.118   1.679  11.402  1.00 43.06 AAAA
ATOM     71  O   THR A  16      -8.728   2.042  12.517  1.00 42.99 AAAA
ATOM     72  N   GLY A  17      -8.453   0.810  10.649  1.00 41.81 AAAA
ATOM     73  CA  GLY A  17      -7.190   0.268  11.109  1.00 40.71 AAAA
ATOM     74  C   GLY A  17      -6.202   1.401  11.275  1.00 39.54 AAAA
ATOM     75  O   GLY A  17      -5.275   1.330  12.085  1.00 39.73 AAAA
ATOM     76  N   GLY A  18      -6.413   2.460  10.500  1.00 37.79 AAAA
ATOM     77  CA  GLY A  18      -5.539   3.611  10.572  1.00 35.68 AAAA
ATOM     78  C   GLY A  18      -5.394   4.116  11.994  1.00 34.88 AAAA
ATOM     79  O   GLY A  18      -4.285   4.441  12.427  1.00 35.21 AAAA
ATOM     80  N   HIS A  19      -6.503   4.186  12.728  1.00 32.89 AAAA
ATOM     81  CA  HIS A  19      -6.454   4.664  14.110  1.00 32.14 AAAA
ATOM     82  CB  HIS A  19      -7.759   5.371  14.504  1.00 30.28 AAAA
ATOM     83  CG  HIS A  19      -8.150   6.504  13.605  1.00 28.85 AAAA
ATOM     84  CD2 HIS A  19      -9.336   6.808  13.027  1.00 27.83 AAAA
ATOM     85  ND1 HIS A  19      -7.288   7.524  13.265  1.00 28.68 AAAA
ATOM     86  CE1 HIS A  19      -7.926   8.407  12.517  1.00 28.09 AAAA
ATOM     87  NE2 HIS A  19      -9.170   7.996  12.358  1.00 27.45 AAAA
ATOM     88  C   HIS A  19      -6.229   3.533  15.108  1.00 31.91 AAAA
ATOM     89  O   HIS A  19      -5.480   3.684  16.072  1.00 31.76 AAAA
ATOM     90  N   VAL A  20      -6.895   2.407  14.881  1.00 31.82 AAAA
ATOM     91  CA  VAL A  20      -6.813   1.271  15.788  1.00 33.08 AAAA
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ATOM     92  CB  VAL A  20      -7.875   0.215  15.430  1.00 33.31 AAAA
ATOM     93  CG1 VAL A  20      -7.766  -0.982  16.361  1.00 33.91 AAAA
ATOM     94  CG2 VAL A  20      -9.260   0.830  15.540  1.00 34.25 AAAA
ATOM     95  C   VAL A  20      -5.452   0.587  15.898  1.00 33.31 AAAA
ATOM     96  O   VAL A  20      -4.977   0.337  17.008  1.00 32.99 AAAA
ATOM     97  N   PHE A  21      -4.823   0.288  14.765  1.00 33.64 AAAA
ATOM     98  CA  PHE A  21      -3.526  -0.385  14.794  1.00 33.68 AAAA
ATOM     99  CB  PHE A  21      -3.020  -0.648  13.368  1.00 35.58 AAAA
ATOM    100  CG  PHE A  21      -3.900  -1.578  12.577  1.00 39.10 AAAA
ATOM    101  CD1 PHE A  21      -4.463  -2.701  13.174  1.00 40.50 AAAA
ATOM    102  CD2 PHE A  21      -4.157  -1.338  11.232  1.00 41.05 AAAA
ATOM    103  CE1 PHE A  21      -5.271  -3.572  12.446  1.00 41.55 AAAA
ATOM    104  CE2 PHE A  21      -4.964  -2.205  10.492  1.00 41.86 AAAA
ATOM    105  CZ  PHE A  21      -5.521  -3.323  11.103  1.00 42.12 AAAA
ATOM    106  C   PHE A  21      -2.456   0.350  15.605  1.00 32.04 AAAA
ATOM    107  O   PHE A  21      -1.789  -0.257  16.443  1.00 31.30 AAAA
ATOM    108  N   PRO A  22      -2.277   1.662  15.375  1.00 31.37 AAAA
ATOM    109  CD  PRO A  22      -2.939   2.544  14.400  1.00 31.41 AAAA
ATOM    110  CA  PRO A  22      -1.259   2.396  16.139  1.00 30.01 AAAA
ATOM    111  CB  PRO A  22      -1.301   3.799  15.536  1.00 30.97 AAAA
ATOM    112  CG  PRO A  22      -1.892   3.592  14.175  1.00 31.19 AAAA
ATOM    113  C   PRO A  22      -1.620   2.411  17.624  1.00 29.31 AAAA
ATOM    114  O   PRO A  22      -0.749   2.366  18.489  1.00 27.42 AAAA
ATOM    115  N   GLY A  23      -2.918   2.483  17.903  1.00 28.99 AAAA
ATOM    116  CA  GLY A  23      -3.380   2.492  19.277  1.00 28.59 AAAA
ATOM    117  C   GLY A  23      -3.035   1.196  19.990  1.00 29.00 AAAA
ATOM    118  O   GLY A  23      -2.649   1.205  21.160  1.00 28.48 AAAA
ATOM    119  N   LEU A  24      -3.168   0.078  19.282  1.00 28.08 AAAA
ATOM    120  CA  LEU A  24      -2.863  -1.227  19.859  1.00 28.39 AAAA
ATOM    121  CB  LEU A  24      -3.306  -2.347  18.913  1.00 28.16 AAAA
ATOM    122  CG  LEU A  24      -4.811  -2.605  18.843  1.00 28.45 AAAA
ATOM    123  CD1 LEU A  24      -5.117  -3.583  17.714  1.00 29.25 AAAA
ATOM    124  CD2 LEU A  24      -5.291  -3.158  20.181  1.00 29.35 AAAA
ATOM    125  C   LEU A  24      -1.373  -1.350  20.147  1.00 28.37 AAAA
ATOM    126  O   LEU A  24      -0.966  -1.986  21.126  1.00 28.60 AAAA
ATOM    127  N   ALA A  25      -0.555  -0.743  19.296  1.00 27.77 AAAA
ATOM    128  CA  ALA A  25       0.887  -0.795  19.497  1.00 28.98 AAAA
ATOM    129  CB  ALA A  25       1.616  -0.142  18.321  1.00 27.53 AAAA
ATOM    130  C   ALA A  25       1.256  -0.093  20.800  1.00 29.10 AAAA
ATOM    131  O   ALA A  25       2.035  -0.618  21.595  1.00 29.49 AAAA
ATOM    132  N   VAL A  26       0.694   1.094  21.020  1.00 28.82 AAAA
ATOM    133  CA  VAL A  26       0.982   1.853  22.233  1.00 28.94 AAAA
ATOM    134  CB  VAL A  26       0.400   3.290  22.157  1.00 29.74 AAAA
ATOM    135  CG1 VAL A  26       0.691   4.049  23.454  1.00 29.76 AAAA
ATOM    136  CG2 VAL A  26       1.009   4.026  20.981  1.00 29.14 AAAA
ATOM    137  C   VAL A  26       0.409   1.131  23.450  1.00 29.18 AAAA
ATOM    138  O   VAL A  26       1.020   1.118  24.518  1.00 29.62 AAAA
ATOM    139  N   ALA A  27      -0.757   0.518  23.286  1.00 27.98 AAAA
ATOM    140  CA  ALA A  27      -1.371  -0.215  24.382  1.00 29.32 AAAA
ATOM    141  CB  ALA A  27      -2.719  -0.755  23.950  1.00 28.32 AAAA
ATOM    142  C   ALA A  27      -0.462  -1.372  24.840  1.00 30.04 AAAA
ATOM    143  O   ALA A  27      -0.084  -1.454  26.015  1.00 29.89 AAAA
ATOM    144  N   HIS A  28      -0.120  -2.259  23.907  1.00 30.92 AAAA
ATOM    145  CA  HIS A  28       0.734  -3.413  24.201  1.00 30.62 AAAA
ATOM    146  CB  HIS A  28       1.024  -4.214  22.924  1.00 30.20 AAAA
ATOM    147  CG  HIS A  28      -0.112  -5.080  22.483  1.00 31.65 AAAA
ATOM    148  CD2 HIS A  28      -0.764  -5.162  21.299  1.00 31.33 AAAA
ATOM    149  ND1 HIS A  28      -0.717  -5.996  23.319  1.00 31.81 AAAA
ATOM    150  CE1 HIS A  28      -1.696  -6.600  22.670  1.00 32.38 AAAA
ATOM    151  NE2 HIS A  28      -1.747  -6.112  21.443  1.00 32.85 AAAA
ATOM    152  C   HIS A  28       2.054  -2.989  24.823  1.00 30.90 AAAA
ATOM    153  O   HIS A  28       2.537  -3.601  25.779  1.00 30.92 AAAA
ATOM    154  N   HIS A  29       2.636  -1.939  24.263  1.00 30.28 AAAA
ATOM    155  CA  HIS A  29       3.899  -1.415  24.742  1.00 30.76 AAAA
ATOM    156  CB  HIS A  29       4.276  -0.195  23.911  1.00 31.40 AAAA
ATOM    157  CG  HIS A  29       5.679   0.274  24.122  1.00 33.14 AAAA
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ATOM    158  CD2 HIS A  29       6.188   1.226  24.939  1.00 33.77 AAAA
ATOM    159  ND1 HIS A  29       6.748  -0.240  23.420  1.00 34.47 AAAA
ATOM    160  CE1 HIS A  29       7.855   0.381  23.791  1.00 34.76 AAAA
ATOM    161  NE2 HIS A  29       7.542   1.275  24.711  1.00 34.09 AAAA
ATOM    162  C   HIS A  29       3.835  -1.032  26.227  1.00 31.63 AAAA
ATOM    163  O   HIS A  29       4.763  -1.315  26.990  1.00 30.76 AAAA
ATOM    164  N   LEU A  30       2.744  -0.388  26.638  1.00 29.72 AAAA
ATOM    165  CA  LEU A  30       2.603   0.035  28.028  1.00 30.08 AAAA
ATOM    166  CB  LEU A  30       1.631   1.225  28.126  1.00 29.45 AAAA
ATOM    167  CG  LEU A  30       2.107   2.503  27.420  1.00 28.69 AAAA
ATOM    168  CD1 LEU A  30       1.026   3.587  27.477  1.00 27.76 AAAA
ATOM    169  CD2 LEU A  30       3.383   2.998  28.075  1.00 28.99 AAAA
ATOM    170  C   LEU A  30       2.153  -1.096  28.950  1.00 30.55 AAAA
ATOM    171  O   LEU A  30       2.538  -1.136  30.120  1.00 31.28 AAAA
ATOM    172  N   MET A  31       1.340  -2.012  28.438  1.00 31.26 AAAA
ATOM    173  CA  MET A  31       0.884  -3.130  29.256  1.00 33.71 AAAA
ATOM    174  CB  MET A  31      -0.118  -3.999  28.494  1.00 34.12 AAAA
ATOM    175  CG  MET A  31      -1.452  -3.341  28.249  1.00 34.98 AAAA
ATOM    176  SD  MET A  31      -2.618  -4.475  27.485  1.00 38.51 AAAA
ATOM    177  CE  MET A  31      -2.086  -4.401  25.803  1.00 37.49 AAAA
ATOM    178  C   MET A  31       2.078  -3.987  29.664  1.00 35.03 AAAA
ATOM    179  O   MET A  31       2.101  -4.548  30.758  1.00 36.09 AAAA
ATOM    180  N   ALA A  32       3.062  -4.085  28.776  1.00 35.62 AAAA
ATOM    181  CA  ALA A  32       4.262  -4.871  29.044  1.00 37.61 AAAA
ATOM    182  CB  ALA A  32       5.049  -5.087  27.755  1.00 37.79 AAAA
ATOM    183  C   ALA A  32       5.133  -4.158  30.070  1.00 38.72 AAAA
ATOM    184  O   ALA A  32       6.223  -4.621  30.409  1.00 39.48 AAAA
ATOM    185  N   GLN A  33       4.654  -3.022  30.560  1.00 38.28 AAAA
ATOM    186  CA  GLN A  33       5.408  -2.275  31.548  1.00 38.14 AAAA
ATOM    187  CB  GLN A  33       5.903  -0.969  30.941  1.00 39.68 AAAA
ATOM    188  CG  GLN A  33       6.856  -1.210  29.791  1.00 42.76 AAAA
ATOM    189  CD  GLN A  33       7.262   0.061  29.096  1.00 44.20 AAAA
ATOM    190  OE1 GLN A  33       7.803   0.975  29.717  1.00 46.28 AAAA
ATOM    191  NE2 GLN A  33       7.002   0.131  27.795  1.00 44.60 AAAA
ATOM    192  C   GLN A  33       4.576  -2.020  32.787  1.00 36.68 AAAA
ATOM    193  O   GLN A  33       4.822  -1.075  33.532  1.00 37.34 AAAA
ATOM    194  N   GLY A  34       3.585  -2.877  33.000  1.00 35.86 AAAA
ATOM    195  CA  GLY A  34       2.738  -2.755  34.170  1.00 35.52 AAAA
ATOM    196  C   GLY A  34       1.461  -1.951  34.008  1.00 34.34 AAAA
ATOM    197  O   GLY A  34       0.611  -1.974  34.897  1.00 33.67 AAAA
ATOM    198  N   TRP A  35       1.314  -1.248  32.890  1.00 34.23 AAAA
ATOM    199  CA  TRP A  35       0.121  -0.435  32.661  1.00 33.63 AAAA
ATOM    200  CB  TRP A  35       0.324   0.509  31.474  1.00 34.84 AAAA
ATOM    201  CG  TRP A  35       1.150   1.722  31.753  1.00 35.09 AAAA
ATOM    202  CD2 TRP A  35       0.722   3.087  31.659  1.00 36.11 AAAA
ATOM    203  CE2 TRP A  35       1.840   3.897  31.957  1.00 36.13 AAAA
ATOM    204  CE3 TRP A  35      -0.499   3.705  31.350  1.00 37.33 AAAA
ATOM    205  CD1 TRP A  35       2.469   1.759  32.099  1.00 35.78 AAAA
ATOM    206  NE1 TRP A  35       2.893   3.062  32.221  1.00 34.49 AAAA
ATOM    207  CZ2 TRP A  35       1.776   5.293  31.955  1.00 37.71 AAAA
ATOM    208  CZ3 TRP A  35      -0.563   5.095  31.348  1.00 37.99 AAAA
ATOM    209  CH2 TRP A  35       0.570   5.874  31.650  1.00 38.17 AAAA
ATOM    210  C   TRP A  35      -1.153  -1.228  32.402  1.00 33.77 AAAA
ATOM    211  O   TRP A  35      -1.136  -2.282  31.763  1.00 32.95 AAAA
ATOM    212  N   GLN A  36      -2.261  -0.704  32.912  1.00 32.90 AAAA
ATOM    213  CA  GLN A  36      -3.567  -1.301  32.696  1.00 33.08 AAAA
ATOM    214  CB  GLN A  36      -4.448  -1.160  33.937  1.00 34.93 AAAA
ATOM    215  CG  GLN A  36      -4.240  -2.228  34.992  1.00 38.58 AAAA
ATOM    216  CD  GLN A  36      -5.272  -2.143  36.103  1.00 40.36 AAAA
ATOM    217  OE1 GLN A  36      -5.295  -1.186  36.874  1.00 42.12 AAAA
ATOM    218  NE2 GLN A  36      -6.140  -3.146  36.181  1.00 42.80 AAAA
ATOM    219  C   GLN A  36      -4.160  -0.482  31.552  1.00 32.42 AAAA
ATOM    220  O   GLN A  36      -4.114   0.748  31.583  1.00 31.42 AAAA
ATOM    221  N   VAL A  37      -4.697  -1.157  30.541  1.00 32.07 AAAA
ATOM    222  CA  VAL A  37      -5.276  -0.456  29.403  1.00 31.91 AAAA
ATOM    223  CB  VAL A  37      -4.436  -0.656  28.123  1.00 32.46 AAAA
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ATOM    224  CG1 VAL A  37      -5.010   0.179  26.983  1.00 32.66 AAAA
ATOM    225  CG2 VAL A  37      -2.994  -0.269  28.379  1.00 31.40 AAAA
ATOM    226  C   VAL A  37      -6.693  -0.917  29.118  1.00 32.15 AAAA
ATOM    227  O   VAL A  37      -7.017  -2.104  29.225  1.00 31.04 AAAA
ATOM    228  N   ARG A  38      -7.532   0.046  28.752  1.00 30.74 AAAA
ATOM    229  CA  ARG A  38      -8.925  -0.202  28.433  1.00 31.08 AAAA
ATOM    230  CB  ARG A  38      -9.807   0.325  29.562  1.00 33.01 AAAA
ATOM    231  CG  ARG A  38     -11.251  -0.116  29.499  1.00 37.13 AAAA
ATOM    232  CD  ARG A  38     -11.532  -1.185  30.529  1.00 39.30 AAAA
ATOM    233  NE  ARG A  38     -12.937  -1.567  30.519  1.00 41.65 AAAA
ATOM    234  CZ  ARG A  38     -13.464  -2.495  31.308  1.00 43.12 AAAA
ATOM    235  NH1 ARG A  38     -12.697  -3.142  32.176  1.00 43.84 AAAA
ATOM    236  NH2 ARG A  38     -14.758  -2.773  31.227  1.00 43.90 AAAA
ATOM    237  C   ARG A  38      -9.196   0.568  27.143  1.00 29.87 AAAA
ATOM    238  O   ARG A  38      -8.574   1.601  26.883  1.00 28.94 AAAA
ATOM    239  N   TRP A  39     -10.119   0.072  26.332  1.00 28.69 AAAA
ATOM    240  CA  TRP A  39     -10.414   0.729  25.071  1.00 28.19 AAAA
ATOM    241  CB  TRP A  39     -10.321  -0.305  23.939  1.00 29.84 AAAA
ATOM    242  CG  TRP A  39     -10.046   0.269  22.583  1.00 33.23 AAAA
ATOM    243  CD2 TRP A  39      -8.774   0.339  21.919  1.00 33.62 AAAA
ATOM    244  CE2 TRP A  39      -8.995   0.945  20.661  1.00 34.00 AAAA
ATOM    245  CE3 TRP A  39      -7.470  -0.052  22.261  1.00 33.80 AAAA
ATOM    246  CD1 TRP A  39     -10.955   0.823  21.729  1.00 34.36 AAAA
ATOM    247  NE1 TRP A  39     -10.332   1.230  20.573  1.00 33.43 AAAA
ATOM    248  CZ2 TRP A  39      -7.960   1.171  19.743  1.00 34.56 AAAA
ATOM    249  CZ3 TRP A  39      -6.442   0.171  21.350  1.00 35.28 AAAA
ATOM    250  CH2 TRP A  39      -6.695   0.779  20.102  1.00 34.47 AAAA
ATOM    251  C   TRP A  39     -11.790   1.395  25.081  1.00 26.35 AAAA
ATOM    252  O   TRP A  39     -12.683   0.994  25.826  1.00 26.68 AAAA
ATOM    253  N   LEU A  40     -11.935   2.438  24.269  1.00 25.04 AAAA
ATOM    254  CA  LEU A  40     -13.197   3.159  24.130  1.00 23.18 AAAA
ATOM    255  CB  LEU A  40     -13.074   4.602  24.637  1.00 22.55 AAAA
ATOM    256  CG  LEU A  40     -14.395   5.381  24.623  1.00 20.79 AAAA
ATOM    257  CD1 LEU A  40     -15.314   4.801  25.675  1.00 21.21 AAAA
ATOM    258  CD2 LEU A  40     -14.149   6.868  24.905  1.00 21.72 AAAA
ATOM    259  C   LEU A  40     -13.495   3.179  22.634  1.00 22.87 AAAA
ATOM    260  O   LEU A  40     -12.718   3.721  21.854  1.00 22.99 AAAA
ATOM    261  N   GLY A  41     -14.608   2.580  22.232  1.00 25.02 AAAA
ATOM    262  CA  GLY A  41     -14.946   2.553  20.821  1.00 25.95 AAAA
ATOM    263  C   GLY A  41     -16.426   2.332  20.594  1.00 28.01 AAAA
ATOM    264  O   GLY A  41     -17.234   2.555  21.494  1.00 28.82 AAAA
ATOM    265  N   THR A  42     -16.783   1.884  19.395  1.00 29.77 AAAA
ATOM    266  CA  THR A  42     -18.185   1.641  19.059  1.00 31.41 AAAA
ATOM    267  CB  THR A  42     -18.603   2.497  17.855  1.00 32.12 AAAA
ATOM    268  OG1 THR A  42     -18.293   3.871  18.119  1.00 34.95 AAAA
ATOM    269  CG2 THR A  42     -20.098   2.367  17.611  1.00 34.55 AAAA
ATOM    270  C   THR A  42     -18.458   0.168  18.741  1.00 32.23 AAAA
ATOM    271  O   THR A  42     -17.721  -0.463  17.986  1.00 29.57 AAAA
ATOM    272  N   ALA A  43     -19.541  -0.360  19.306  1.00 34.77 AAAA
ATOM    273  CA  ALA A  43     -19.920  -1.760  19.127  1.00 37.23 AAAA
ATOM    274  CB  ALA A  43     -21.173  -2.060  19.948  1.00 37.66 AAAA
ATOM    275  C   ALA A  43     -20.126  -2.232  17.686  1.00 39.10 AAAA
ATOM    276  O   ALA A  43     -20.088  -3.434  17.422  1.00 39.09 AAAA
ATOM    277  N   ASP A  44     -20.333  -1.304  16.757  1.00 40.78 AAAA
ATOM    278  CA  ASP A  44     -20.557  -1.671  15.361  1.00 42.78 AAAA
ATOM    279  CB  ASP A  44     -21.678  -0.812  14.774  1.00 44.80 AAAA
ATOM    280  CG  ASP A  44     -21.438   0.670  14.973  1.00 46.37 AAAA
ATOM    281  OD1 ASP A  44     -20.464   1.206  14.400  1.00 48.22 AAAA
ATOM    282  OD2 ASP A  44     -22.220   1.302  15.712  1.00 49.14 AAAA
ATOM    283  C   ASP A  44     -19.324  -1.559  14.472  1.00 43.14 AAAA
ATOM    284  O   ASP A  44     -19.320  -2.061  13.349  1.00 44.14 AAAA
ATOM    285  N   ARG A  45     -18.281  -0.904  14.970  1.00 42.77 AAAA
ATOM    286  CA  ARG A  45     -17.056  -0.730  14.199  1.00 42.34 AAAA
ATOM    287  CB  ARG A  45     -16.415   0.614  14.550  1.00 44.43 AAAA
ATOM    288  CG  ARG A  45     -17.206   1.822  14.056  1.00 48.23 AAAA
ATOM    289  CD  ARG A  45     -17.272   1.845  12.533  1.00 51.20 AAAA
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ATOM    290  NE  ARG A  45     -17.950    3.029   12.014  1.00 54.35 AAAA
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ATOM    292  NH1 ARG A  45     -16.417    4.522   12.881  1.00 56.45 AAAA
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ATOM    299  CG  MET A  46     -12.239   -1.544   12.423  1.00 42.15 AAAA
ATOM    300  SD  MET A  46     -10.690   -1.620   13.352  1.00 44.74 AAAA
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ATOM    306  CB  GLU A  47     -12.309   -0.820   17.650  1.00 35.19 AAAA
ATOM    307  CG  GLU A  47     -13.615   -0.150   18.058  1.00 34.12 AAAA
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ATOM    310  OE2 GLU A  47     -14.995    1.652   17.350  1.00 32.08 AAAA
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ATOM    337  CG1 VAL A  51      -9.571   -3.795   22.523  1.00 35.15 AAAA
ATOM    338  CG2 VAL A  51      -9.810   -2.777   20.256  1.00 34.42 AAAA
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ATOM    353  CE  LYS A  53     -11.280  -12.102   16.133  1.00 45.87 AAAA
ATOM    354  NZ  LYS A  53     -11.250  -12.342   14.659  1.00 47.88 AAAA
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ATOM    411  CE2 PHE A  60     -17.042  -2.104  21.397  1.00 34.93 AAAA
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ATOM	506	CA	ALA	A	73	-23.282	15.650	12.954	1.00	39.79	AAAA
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ATOM    576  CE1 PHE A  82     -25.430  16.831  29.916  1.00 20.18 AAAA
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ATOM    688  OH  TYR A  95      -7.120   0.687  32.019  1.00 33.09 AAAA
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ATOM    693  CB  LYS A  96     -10.543   5.658  37.966  1.00 32.14 AAAA
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ATOM    718  CG1 VAL A  99      -2.684   8.220  30.614  1.00 25.72 AAAA
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ATOM    724  CB  VAL A 100      -8.038   9.451  27.663  1.00 21.17 AAAA
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ATOM    728  O   VAL A 100      -5.244  10.505  26.464  1.00 21.01 AAAA
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ATOM    737  N   GLY A 102      -6.127   9.742  22.484  1.00 21.18 AAAA
ATOM    738  CA  GLY A 102      -7.043   9.780  21.358  1.00 21.84 AAAA
ATOM    739  C   GLY A 102      -6.246   9.586  20.079  1.00 21.20 AAAA
ATOM    740  O   GLY A 102      -5.294  10.324  19.837  1.00 22.62 AAAA
ATOM    741  N   MET A 103      -6.627   8.599  19.270  1.00 21.18 AAAA
ATOM    742  CA  MET A 103      -5.933   8.312  18.015  1.00 22.83 AAAA
ATOM    743  CB  MET A 103      -5.715   6.805  17.865  1.00 23.16 AAAA
ATOM    744  CG  MET A 103      -4.978   6.140  19.030  1.00 24.31 AAAA
ATOM    745  SD  MET A 103      -3.333   6.804  19.308  1.00 27.62 AAAA
ATOM    746  CE  MET A 103      -2.455   6.156  17.873  1.00 26.43 AAAA
ATOM    747  C   MET A 103      -6.709   8.823  16.795  1.00 23.47 AAAA
ATOM    748  O   MET A 103      -6.351   8.532  15.653  1.00 23.75 AAAA
ATOM    749  N   GLY A 104      -7.767   9.590  17.043  1.00 25.38 AAAA
ATOM    750  CA  GLY A 104      -8.585  10.114  15.959  1.00 25.56 AAAA
ATOM    751  C   GLY A 104      -9.878   9.326  15.833  1.00 25.55 AAAA
ATOM    752  O   GLY A 104     -10.004   8.241  16.404  1.00 26.58 AAAA
ATOM    753  N   GLY A 105     -10.840   9.854  15.082  1.00 26.06 AAAA
ATOM    754  CA  GLY A 105     -12.107   9.159  14.930  1.00 26.21 AAAA
ATOM    755  C   GLY A 105     -13.140   9.819  15.823  1.00 26.96 AAAA
ATOM    756  O   GLY A 105     -12.810  10.258  16.926  1.00 25.49 AAAA
ATOM    757  N   TYR A 106     -14.393   9.863  15.376  1.00 27.65 AAAA
ATOM    758  CA  TYR A 106     -15.434  10.534  16.145  1.00 28.10 AAAA
ATOM    759  CB  TYR A 106     -16.759  10.556  15.362  1.00 31.05 AAAA
ATOM    760  CG  TYR A 106     -17.536   9.257  15.303  1.00 33.49 AAAA
ATOM    761  CD1 TYR A 106     -18.269   8.802  16.400  1.00 34.81 AAAA
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ATOM    762  CE1 TYR A 106     -19.038   7.634  16.323  1.00 36.18 AAAA
ATOM    763  CD2 TYR A 106     -17.581   8.509  14.123  1.00 35.64 AAAA
ATOM    764  CE2 TYR A 106     -18.343   7.344  14.032  1.00 36.47 AAAA
ATOM    765  CZ  TYR A 106     -19.069   6.912  15.133  1.00 37.27 AAAA
ATOM    766  OH  TYR A 106     -19.829   5.766  15.027  1.00 38.99 AAAA
ATOM    767  C   TYR A 106     -15.678  10.072  17.576  1.00 26.46 AAAA
ATOM    768  O   TYR A 106     -15.976  10.897  18.430  1.00 26.55 AAAA
ATOM    769  N   VAL A 107     -15.549   8.780  17.858  1.00 25.31 AAAA
ATOM    770  CA  VAL A 107     -15.783   8.318  19.223  1.00 23.91 AAAA
ATOM    771  CB  VAL A 107     -15.659   6.772  19.335  1.00 25.47 AAAA
ATOM    772  CG1 VAL A 107     -14.224   6.327  19.076  1.00 26.57 AAAA
ATOM    773  CG2 VAL A 107     -16.126   6.315  20.711  1.00 24.96 AAAA
ATOM    774  C   VAL A 107     -14.836   8.993  20.223  1.00 23.22 AAAA
ATOM    775  O   VAL A 107     -15.190   9.190  21.389  1.00 23.17 AAAA
ATOM    776  N   SER A 108     -13.650   9.381  19.765  1.00 23.13 AAAA
ATOM    777  CA  SER A 108     -12.676  10.029  20.643  1.00 23.40 AAAA
ATOM    778  CB  SER A 108     -11.301  10.108  19.967  1.00 23.85 AAAA
ATOM    779  OG  SER A 108     -11.292  11.038  18.899  1.00 25.04 AAAA
ATOM    780  C   SER A 108     -13.121  11.430  21.044  1.00 23.03 AAAA
ATOM    781  O   SER A 108     -12.592  12.009  21.993  1.00 22.32 AAAA
ATOM    782  N   GLY A 109     -14.089  11.979  20.310  1.00 21.84 AAAA
ATOM    783  CA  GLY A 109     -14.583  13.307  20.627  1.00 21.98 AAAA
ATOM    784  C   GLY A 109     -15.297  13.342  21.972  1.00 20.30 AAAA
ATOM    785  O   GLY A 109     -14.898  14.088  22.856  1.00 21.37 AAAA
ATOM    786  N   PRO A 110     -16.369  12.557  22.155  1.00 20.07 AAAA
ATOM    787  CD  PRO A 110     -16.992  11.637  21.191  1.00 20.80 AAAA
ATOM    788  CA  PRO A 110     -17.085  12.550  23.436  1.00 19.58 AAAA
ATOM    789  CB  PRO A 110     -18.232  11.569  23.199  1.00 20.85 AAAA
ATOM    790  CG  PRO A 110     -18.398  11.548  21.702  1.00 22.43 AAAA
ATOM    791  C   PRO A 110     -16.136  12.031  24.524  1.00 18.52 AAAA
ATOM    792  O   PRO A 110     -16.184  12.462  25.675  1.00 19.12 AAAA
ATOM    793  N   GLY A 111     -15.286  11.086  24.140  1.00 19.12 AAAA
ATOM    794  CA  GLY A 111     -14.332  10.525  25.087  1.00 18.87 AAAA
ATOM    795  C   GLY A 111     -13.402  11.601  25.612  1.00 17.97 AAAA
ATOM    796  O   GLY A 111     -13.208  11.730  26.813  1.00 19.32 AAAA
ATOM    797  N   GLY A 112     -12.822  12.380  24.704  1.00 18.62 AAAA
ATOM    798  CA  GLY A 112     -11.925  13.451  25.105  1.00 17.38 AAAA
ATOM    799  C   GLY A 112     -12.610  14.509  25.957  1.00 17.36 AAAA
ATOM    800  O   GLY A 112     -12.035  14.997  26.936  1.00 16.49 AAAA
ATOM    801  N   LEU A 113     -13.837  14.864  25.583  1.00 16.45 AAAA
ATOM    802  CA  LEU A 113     -14.611  15.866  26.314  1.00 17.35 AAAA
ATOM    803  CB  LEU A 113     -15.974  16.079  25.640  1.00 17.68 AAAA
ATOM    804  CG  LEU A 113     -16.735  17.409  25.805  1.00 21.99 AAAA
ATOM    805  CD1 LEU A 113     -18.205  17.154  25.511  1.00 20.80 AAAA
ATOM    806  CD2 LEU A 113     -16.570  18.007  27.178  1.00 22.94 AAAA
ATOM    807  C   LEU A 113     -14.836  15.329  27.725  1.00 16.05 AAAA
ATOM    808  O   LEU A 113     -14.695  16.045  28.711  1.00 16.63 AAAA
ATOM    809  N   ALA A 114     -15.199  14.056  27.801  1.00 16.59 AAAA
ATOM    810  CA  ALA A 114     -15.442  13.416  29.087  1.00 15.95 AAAA
ATOM    811  CB  ALA A 114     -15.859  11.963  28.868  1.00 17.72 AAAA
ATOM    812  C   ALA A 114     -14.194  13.492  29.968  1.00 15.37 AAAA
ATOM    813  O   ALA A 114     -14.260  13.952  31.105  1.00 15.94 AAAA
ATOM    814  N   ALA A 115     -13.053  13.050  29.452  1.00 16.63 AAAA
ATOM    815  CA  ALA A 115     -11.820  13.098  30.251  1.00 15.65 AAAA
ATOM    816  CB  ALA A 115     -10.641  12.518  29.450  1.00 15.52 AAAA
ATOM    817  C   ALA A 115     -11.506  14.530  30.693  1.00 16.10 AAAA
ATOM    818  O   ALA A 115     -11.141  14.777  31.841  1.00 15.67 AAAA
ATOM    819  N   TRP A 116     -11.650  15.480  29.778  1.00 16.71 AAAA
ATOM    820  CA  TRP A 116     -11.380  16.873  30.100  1.00 17.31 AAAA
ATOM    821  CB  TRP A 116     -11.542  17.723  28.835  1.00 18.91 AAAA
ATOM    822  CG  TRP A 116     -11.172  19.155  29.003  1.00 21.69 AAAA
ATOM    823  CD2 TRP A 116     -12.008  20.277  28.740  1.00 23.65 AAAA
ATOM    824  CE2 TRP A 116     -11.262  21.438  29.048  1.00 25.14 AAAA
ATOM    825  CE3 TRP A 116     -13.321  20.418  28.268  1.00 26.49 AAAA
ATOM    826  CD1 TRP A 116      -9.979  19.658  29.447  1.00 23.00 AAAA
ATOM    827  NE1 TRP A 116     -10.025  21.032  29.479  1.00 24.96 AAAA
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ATOM    828  CZ2 TRP A 116     -11.785  22.724  28.902  1.00 26.16 AAAA
ATOM    829  CZ3 TRP A 116     -13.842  21.702  28.122  1.00 26.44 AAAA
ATOM    830  CH2 TRP A 116     -13.072  22.834  28.439  1.00 25.35 AAAA
ATOM    831  C   TRP A 116     -12.292  17.377  31.233  1.00 16.50 AAAA
ATOM    832  O   TRP A 116     -11.835  18.080  32.137  1.00 16.03 AAAA
ATOM    833  N   SER A 117     -13.565  16.990  31.200  1.00 16.73 AAAA
ATOM    834  CA  SER A 117     -14.528  17.399  32.229  1.00 17.06 AAAA
ATOM    835  CB  SER A 117     -15.961  17.116  31.762  1.00 16.18 AAAA
ATOM    836  OG  SER A 117     -16.270  15.731  31.743  1.00 18.31 AAAA
ATOM    837  C   SER A 117     -14.289  16.720  33.586  1.00 18.05 AAAA
ATOM    838  O   SER A 117     -14.837  17.147  34.605  1.00 17.79 AAAA
ATOM    839  N   LEU A 118     -13.466  15.678  33.594  1.00 18.13 AAAA
ATOM    840  CA  LEU A 118     -13.146  14.950  34.827  1.00 19.26 AAAA
ATOM    841  CB  LEU A 118     -13.262  13.441  34.587  1.00 18.09 AAAA
ATOM    842  CG  LEU A 118     -14.686  12.932  34.353  1.00 20.04 AAAA
ATOM    843  CD1 LEU A 118     -14.659  11.484  33.869  1.00 20.30 AAAA
ATOM    844  CD2 LEU A 118     -15.480  13.064  35.646  1.00 20.40 AAAA
ATOM    845  C   LEU A 118     -11.736  15.283  35.305  1.00 20.78 AAAA
ATOM    846  O   LEU A 118     -11.267  14.763  36.321  1.00 20.64 AAAA
ATOM    847  N   GLY A 119     -11.057  16.152  34.566  1.00 21.27 AAAA
ATOM    848  CA  GLY A 119      -9.706  16.537  34.943  1.00 21.97 AAAA
ATOM    849  C   GLY A 119      -8.648  15.519  34.550  1.00 21.55 AAAA
ATOM    850  O   GLY A 119      -7.515  15.582  35.034  1.00 21.92 AAAA
ATOM    851  N   ILE A 120      -9.009  14.584  33.678  1.00 20.43 AAAA
ATOM    852  CA  ILE A 120      -8.082  13.548  33.214  1.00 21.09 AAAA
ATOM    853  CB  ILE A 120      -8.853  12.270  32.836  1.00 20.95 AAAA
ATOM    854  CG2 ILE A 120      -7.902  11.226  32.275  1.00 22.20 AAAA
ATOM    855  CG1 ILE A 120      -9.624  11.748  34.051  1.00 22.05 AAAA
ATOM    856  CD1 ILE A 120     -10.688  10.709  33.689  1.00 21.95 AAAA
ATOM    857  C   ILE A 120      -7.358  14.088  31.978  1.00 20.81 AAAA
ATOM    858  O   ILE A 120      -8.001  14.465  31.004  1.00 21.35 AAAA
ATOM    859  N   PRO A 121      -6.013  14.131  31.999  1.00 20.67 AAAA
ATOM    860  CD  PRO A 121      -5.052  13.722  33.040  1.00 20.88 AAAA
ATOM    861  CA  PRO A 121      -5.320  14.658  30.819  1.00 20.52 AAAA
ATOM    862  CB  PRO A 121      -3.842  14.649  31.237  1.00 21.37 AAAA
ATOM    863  CG  PRO A 121      -3.777  13.532  32.240  1.00 22.04 AAAA
ATOM    864  C   PRO A 121      -5.580  13.893  29.536  1.00 19.38 AAAA
ATOM    865  O   PRO A 121      -5.717  12.671  29.538  1.00 18.17 AAAA
ATOM    866  N   VAL A 122      -5.647  14.645  28.442  1.00 20.01 AAAA
ATOM    867  CA  VAL A 122      -5.903  14.102  27.120  1.00 19.76 AAAA
ATOM    868  CB  VAL A 122      -7.047  14.866  26.421  1.00 18.63 AAAA
ATOM    869  CG1 VAL A 122      -7.286  14.281  25.033  1.00 20.46 AAAA
ATOM    870  CG2 VAL A 122      -8.320  14.790  27.264  1.00 20.31 AAAA
ATOM    871  C   VAL A 122      -4.672  14.205  26.223  1.00 19.39 AAAA
ATOM    872  O   VAL A 122      -4.096  15.282  26.069  1.00 19.66 AAAA
ATOM    873  N   VAL A 123      -4.284  13.079  25.634  1.00 19.86 AAAA
ATOM    874  CA  VAL A 123      -3.134  13.029  24.734  1.00 20.22 AAAA
ATOM    875  CB  VAL A 123      -2.086  11.982  25.200  1.00 20.59 AAAA
ATOM    876  CG1 VAL A 123      -0.898  11.957  24.226  1.00 20.51 AAAA
ATOM    877  CG2 VAL A 123      -1.602  12.317  26.606  1.00 17.21 AAAA
ATOM    878  C   VAL A 123      -3.684  12.600  23.381  1.00 21.06 AAAA
ATOM    879  O   VAL A 123      -4.482  11.666  23.300  1.00 22.10 AAAA
ATOM    880  N   LEU A 124      -3.269  13.284  22.325  1.00 21.08 AAAA
ATOM    881  CA  LEU A 124      -3.746  12.952  20.989  1.00 21.68 AAAA
ATOM    882  CB  LEU A 124      -4.463  14.149  20.366  1.00 21.81 AAAA
ATOM    883  CG  LEU A 124      -5.629  14.805  21.105  1.00 21.93 AAAA
ATOM    884  CD1 LEU A 124      -6.133  15.980  20.268  1.00 22.15 AAAA
ATOM    885  CD2 LEU A 124      -6.737  13.787  21.337  1.00 21.49 AAAA
ATOM    886  C   LEU A 124      -2.628  12.558  20.038  1.00 21.67 AAAA
ATOM    887  O   LEU A 124      -1.493  13.011  20.170  1.00 22.39 AAAA
ATOM    888  N   HIS A 125      -2.964  11.713  19.075  1.00 22.63 AAAA
ATOM    889  CA  HIS A 125      -2.014  11.336  18.036  1.00 24.74 AAAA
ATOM    890  CB  HIS A 125      -1.429   9.939  18.244  1.00 24.62 AAAA
ATOM    891  CG  HIS A 125      -0.471   9.540  17.162  1.00 27.30 AAAA
ATOM    892  CD2 HIS A 125      -0.629   8.744  16.079  1.00 27.23 AAAA
ATOM    893  ND1 HIS A 125       0.806  10.057  17.072  1.00 29.96 AAAA
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ATOM    894  CE1 HIS A 125       1.391   9.597  15.979  1.00 27.40 AAAA
ATOM    895  NE2 HIS A 125       0.541   8.799  15.358  1.00 28.94 AAAA
ATOM    896  C   HIS A 125      -2.763  11.364  16.705  1.00 24.38 AAAA
ATOM    897  O   HIS A 125      -3.813  10.741  16.565  1.00 23.93 AAAA
ATOM    898  N   GLU A 126      -2.233  12.111  15.744  1.00 24.36 AAAA
ATOM    899  CA  GLU A 126      -2.836  12.199  14.420  1.00 26.31 AAAA
ATOM    900  CB  GLU A 126      -2.992  13.664  14.005  1.00 25.81 AAAA
ATOM    901  CG  GLU A 126      -3.465  13.861  12.567  1.00 26.62 AAAA
ATOM    902  CD  GLU A 126      -4.795  13.196  12.288  1.00 27.69 AAAA
ATOM    903  OE1 GLU A 126      -5.785  13.544  12.965  1.00 27.90 AAAA
ATOM    904  OE2 GLU A 126      -4.855  12.326  11.391  1.00 27.53 AAAA
ATOM    905  C   GLU A 126      -1.901  11.472  13.456  1.00 27.49 AAAA
ATOM    906  O   GLU A 126      -0.727  11.819  13.349  1.00 27.87 AAAA
ATOM    907  N   GLN A 127      -2.423  10.463  12.765  1.00 28.80 AAAA
ATOM    908  CA  GLN A 127      -1.617   9.682  11.834  1.00 30.09 AAAA
ATOM    909  CB  GLN A 127      -2.192   8.264  11.688  1.00 28.89 AAAA
ATOM    910  CG  GLN A 127      -2.184   7.421  12.958  1.00 28.94 AAAA
ATOM    911  CD  GLN A 127      -3.456   7.578  13.775  1.00 29.34 AAAA
ATOM    912  OE1 GLN A 127      -4.543   7.207  13.329  1.00 29.36 AAAA
ATOM    913  NE2 GLN A 127      -3.326   8.131  14.973  1.00 28.70 AAAA
ATOM    914  C   GLN A 127      -1.455  10.277  10.438  1.00 30.92 AAAA
ATOM    915  O   GLN A 127      -0.428  10.068   9.794  1.00 31.21 AAAA
ATOM    916  N   ASN A 128      -2.448  11.038   9.986  1.00 32.48 AAAA
ATOM    917  CA  ASN A 128      -2.434  11.596   8.634  1.00 33.12 AAAA
ATOM    918  CB  ASN A 128      -3.864  11.589   8.083  1.00 32.20 AAAA
ATOM    919  CG  ASN A 128      -4.606  10.312   8.424  1.00 33.05 AAAA
ATOM    920  OD1 ASN A 128      -5.296  10.236   9.445  1.00 33.34 AAAA
ATOM    921  ND2 ASN A 128      -4.454   9.292   7.584  1.00 31.22 AAAA
ATOM    922  C   ASN A 128      -1.809  12.971   8.394  1.00 33.60 AAAA
ATOM    923  O   ASN A 128      -1.571  13.744   9.327  1.00 34.03 AAAA
ATOM    924  N   GLY A 129      -1.550  13.256   7.117  1.00 33.69 AAAA
ATOM    925  CA  GLY A 129      -0.959  14.524   6.718  1.00 33.68 AAAA
ATOM    926  C   GLY A 129      -1.903  15.682   6.972  1.00 33.41 AAAA
ATOM    927  O   GLY A 129      -1.482  16.834   7.057  1.00 32.92 AAAA
ATOM    928  N   ILE A 130      -3.192  15.374   7.070  1.00 33.49 AAAA
ATOM    929  CA  ILE A 130      -4.205  16.383   7.361  1.00 33.06 AAAA
ATOM    930  CB  ILE A 130      -5.204  16.570   6.206  1.00 33.49 AAAA
ATOM    931  CG2 ILE A 130      -4.548  17.358   5.083  1.00 35.66 AAAA
ATOM    932  CG1 ILE A 130      -5.736  15.209   5.751  1.00 34.45 AAAA
ATOM    933  CD1 ILE A 130      -6.775  15.279   4.665  1.00 35.68 AAAA
ATOM    934  C   ILE A 130      -4.964  15.892   8.584  1.00 32.19 AAAA
ATOM    935  O   ILE A 130      -5.379  14.733   8.644  1.00 32.07 AAAA
ATOM    936  N   ALA A 131      -5.135  16.771   9.561  1.00 31.26 AAAA
ATOM    937  CA  ALA A 131      -5.832  16.404  10.788  1.00 30.63 AAAA
ATOM    938  CB  ALA A 131      -5.735  17.547  11.800  1.00 30.70 AAAA
ATOM    939  C   ALA A 131      -7.292  16.038  10.556  1.00 30.27 AAAA
ATOM    940  O   ALA A 131      -7.992  16.682   9.774  1.00 30.54 AAAA
ATOM    941  N   GLY A 132      -7.743  14.987  11.232  1.00 29.03 AAAA
ATOM    942  CA  GLY A 132      -9.131  14.587  11.119  1.00 27.98 AAAA
ATOM    943  C   GLY A 132      -9.902  15.678  11.837  1.00 26.80 AAAA
ATOM    944  O   GLY A 132      -9.326  16.387  12.660  1.00 25.68 AAAA
ATOM    945  N   LEU A 133     -11.188  15.827  11.543  1.00 26.51 AAAA
ATOM    946  CA  LEU A 133     -11.973  16.882  12.186  1.00 26.70 AAAA
ATOM    947  CB  LEU A 133     -13.363  16.967  11.538  1.00 28.16 AAAA
ATOM    948  CG  LEU A 133     -14.275  18.138  11.936  1.00 28.52 AAAA
ATOM    949  CD1 LEU A 133     -14.889  17.874  13.280  1.00 32.18 AAAA
ATOM    950  CD2 LEU A 133     -13.486  19.436  11.960  1.00 30.27 AAAA
ATOM    951  C   LEU A 133     -12.097  16.713  13.703  1.00 25.88 AAAA
ATOM    952  O   LEU A 133     -12.063  17.700  14.444  1.00 26.12 AAAA
ATOM    953  N   THR A 134     -12.240  15.475  14.169  1.00 24.18 AAAA
ATOM    954  CA  THR A 134     -12.353  15.230  15.608  1.00 23.78 AAAA
ATOM    955  CB  THR A 134     -12.605  13.729  15.922  1.00 23.18 AAAA
ATOM    956  OG1 THR A 134     -13.814  13.300  15.285  1.00 23.74 AAAA
ATOM    957  CG2 THR A 134     -12.751  13.511  17.433  1.00 23.66 AAAA
ATOM    958  C   THR A 134     -11.071  15.671  16.315  1.00 22.68 AAAA
ATOM    959  O   THR A 134     -11.116  16.368  17.328  1.00 21.38 AAAA
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ATOM    960  N   ASN A 135      -9.927  15.267  15.771  1.00 23.98 AAAA
ATOM    961  CA  ASN A 135      -8.636  15.623  16.358  1.00 24.64 AAAA
ATOM    962  CB  ASN A 135      -7.488  14.936  15.597  1.00 24.49 AAAA
ATOM    963  CG  ASN A 135      -7.020  13.638  16.264  1.00 25.25 AAAA
ATOM    964  OD1 ASN A 135      -6.267  12.856  15.668  1.00 25.70 AAAA
ATOM    965  ND2 ASN A 135      -7.445  13.415  17.504  1.00 22.51 AAAA
ATOM    966  C   ASN A 135      -8.421  17.135  16.349  1.00 25.19 AAAA
ATOM    967  O   ASN A 135      -7.890  17.702  17.301  1.00 24.79 AAAA
ATOM    968  N   LYS A 136      -8.839  17.792  15.274  1.00 26.78 AAAA
ATOM    969  CA  LYS A 136      -8.661  19.234  15.177  1.00 28.71 AAAA
ATOM    970  CB  LYS A 136      -9.165  19.743  13.828  1.00 30.84 AAAA
ATOM    971  CG  LYS A 136      -8.816  21.195  13.563  1.00 34.68 AAAA
ATOM    972  CD  LYS A 136      -9.206  21.596  12.148  1.00 36.19 AAAA
ATOM    973  CE  LYS A 136      -8.810  23.033  11.846  1.00 37.78 AAAA
ATOM    974  NZ  LYS A 136      -9.124  23.414  10.432  1.00 40.33 AAAA
ATOM    975  C   LYS A 136      -9.370  19.981  16.304  1.00 28.66 AAAA
ATOM    976  O   LYS A 136      -8.803  20.900  16.902  1.00 28.47 AAAA
ATOM    977  N   TRP A 137     -10.606  19.589  16.596  1.00 28.05 AAAA
ATOM    978  CA  TRP A 137     -11.363  20.243  17.656  1.00 28.85 AAAA
ATOM    979  CB  TRP A 137     -12.855  19.921  17.516  1.00 31.86 AAAA
ATOM    980  CG  TRP A 137     -13.485  20.502  16.282  1.00 34.71 AAAA
ATOM    981  CD2 TRP A 137     -14.788  20.206  15.755  1.00 36.70 AAAA
ATOM    982  CE2 TRP A 137     -14.982  21.036  14.630  1.00 37.21 AAAA
ATOM    983  CE3 TRP A 137     -15.811  19.321  16.130  1.00 38.46 AAAA
ATOM    984  CD1 TRP A 137     -12.959  21.466  15.471  1.00 36.22 AAAA
ATOM    985  NE1 TRP A 137     -13.851  21.794  14.480  1.00 36.96 AAAA
ATOM    986  CZ2 TRP A 137     -16.160  21.010  13.869  1.00 38.57 AAAA
ATOM    987  CZ3 TRP A 137     -16.986  19.295  15.373  1.00 39.12 AAAA
ATOM    988  CH2 TRP A 137     -17.148  20.136  14.255  1.00 39.31 AAAA
ATOM    989  C   TRP A 137     -10.868  19.803  19.029  1.00 28.01 AAAA
ATOM    990  O   TRP A 137     -10.763  20.605  19.955  1.00 27.04 AAAA
ATOM    991  N   LEU A 138     -10.548  18.520  19.143  1.00 27.31 AAAA
ATOM    992  CA  LEU A 138     -10.072  17.943  20.393  1.00 26.35 AAAA
ATOM    993  CB  LEU A 138      -9.879  16.444  20.174  1.00 27.79 AAAA
ATOM    994  CG  LEU A 138     -10.054  15.384  21.262  1.00 30.24 AAAA
ATOM    995  CD1 LEU A 138     -11.263  15.650  22.142  1.00 29.67 AAAA
ATOM    996  CD2 LEU A 138     -10.178  14.036  20.562  1.00 30.06 AAAA
ATOM    997  C   LEU A 138      -8.772  18.609  20.834  1.00 25.34 AAAA
ATOM    998  O   LEU A 138      -8.532  18.814  22.030  1.00 23.81 AAAA
ATOM    999  N   ALA A 139      -7.931  18.953  19.865  1.00 26.03 AAAA
ATOM   1000  CA  ALA A 139      -6.657  19.595  20.160  1.00 26.05 AAAA
ATOM   1001  CB  ALA A 139      -5.918  19.934  18.858  1.00 26.98 AAAA
ATOM   1002  C   ALA A 139      -6.847  20.858  21.002  1.00 26.86 AAAA
ATOM   1003  O   ALA A 139      -5.929  21.286  21.697  1.00 26.11 AAAA
ATOM   1004  N   LYS A 140      -8.044  21.439  20.952  1.00 26.32 AAAA
ATOM   1005  CA  LYS A 140      -8.329  22.649  21.716  1.00 26.90 AAAA
ATOM   1006  CB  LYS A 140      -9.644  23.276  21.238  1.00 29.14 AAAA
ATOM   1007  CG  LYS A 140      -9.665  23.595  19.749  1.00 31.62 AAAA
ATOM   1008  CD  LYS A 140      -8.523  24.513  19.364  1.00 35.02 AAAA
ATOM   1009  CE  LYS A 140      -8.811  25.975  19.704  1.00 37.44 AAAA
ATOM   1010  NZ  LYS A 140      -9.865  26.555  18.812  1.00 40.43 AAAA
ATOM   1011  C   LYS A 140      -8.395  22.414  23.230  1.00 25.59 AAAA
ATOM   1012  O   LYS A 140      -8.333  23.361  24.004  1.00 24.94 AAAA
ATOM   1013  N   ILE A 141      -8.526  21.159  23.649  1.00 24.13 AAAA
ATOM   1014  CA  ILE A 141      -8.587  20.844  25.075  1.00 23.31 AAAA
ATOM   1015  CB  ILE A 141      -9.971  20.270  25.477  1.00 22.85 AAAA
ATOM   1016  CG2 ILE A 141     -11.046  21.355  25.372  1.00 23.88 AAAA
ATOM   1017  CG1 ILE A 141     -10.313  19.071  24.595  1.00 23.34 AAAA
ATOM   1018  CD1 ILE A 141     -11.574  18.339  25.012  1.00 25.61 AAAA
ATOM   1019  C   ILE A 141      -7.524  19.822  25.482  1.00 23.06 AAAA
ATOM   1020  O   ILE A 141      -7.427  19.450  26.655  1.00 22.52 AAAA
ATOM   1021  N   ALA A 142      -6.724  19.375  24.520  1.00 21.80 AAAA
ATOM   1022  CA  ALA A 142      -5.695  18.379  24.803  1.00 21.97 AAAA
ATOM   1023  CB  ALA A 142      -5.231  17.739  23.495  1.00 20.41 AAAA
ATOM   1024  C   ALA A 142      -4.491  18.924  25.580  1.00 21.11 AAAA
ATOM   1025  O   ALA A 142      -4.132  20.094  25.465  1.00 22.76 AAAA
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ATOM   1026  N   THR A 143      -3.887  18.056  26.384  1.00 21.92 AAAA
ATOM   1027  CA  THR A 143      -2.707  18.391  27.178  1.00 22.64 AAAA
ATOM   1028  CB  THR A 143      -2.598  17.450  28.400  1.00 23.91 AAAA
ATOM   1029  OG1 THR A 143      -3.751  17.635  29.232  1.00 25.42 AAAA
ATOM   1030  CG2 THR A 143      -1.329  17.735  29.209  1.00 24.48 AAAA
ATOM   1031  C   THR A 143      -1.454  18.235  26.312  1.00 22.79 AAAA
ATOM   1032  O   THR A 143      -0.444  18.910  26.517  1.00 23.30 AAAA
ATOM   1033  N   LYS A 144      -1.525  17.341  25.335  1.00 23.20 AAAA
ATOM   1034  CA  LYS A 144      -0.398  17.106  24.440  1.00 25.09 AAAA
ATOM   1035  CB  LYS A 144       0.565  16.083  25.049  1.00 25.01 AAAA
ATOM   1036  CG  LYS A 144       1.706  15.658  24.129  1.00 28.28 AAAA
ATOM   1037  CD  LYS A 144       2.604  16.838  23.747  1.00 27.48 AAAA
ATOM   1038  CE  LYS A 144       3.818  16.373  22.946  1.00 29.11 AAAA
ATOM   1039  NZ  LYS A 144       4.722  17.507  22.587  1.00 28.97 AAAA
ATOM   1040  C   LYS A 144      -0.896  16.595  23.102  1.00 24.77 AAAA
ATOM   1041  O   LYS A 144      -1.688  15.660  23.039  1.00 24.45 AAAA
ATOM   1042  N   VAL A 145      -0.432  17.218  22.030  1.00 24.92 AAAA
ATOM   1043  CA  VAL A 145      -0.830  16.793  20.701  1.00 25.14 AAAA
ATOM   1044  CB  VAL A 145      -1.510  17.938  19.919  1.00 24.18 AAAA
ATOM   1045  CG1 VAL A 145      -2.023  17.418  18.591  1.00 24.71 AAAA
ATOM   1046  CG2 VAL A 145      -2.658  18.528  20.740  1.00 25.82 AAAA
ATOM   1047  C   VAL A 145       0.420  16.356  19.950  1.00 25.49 AAAA
ATOM   1048  O   VAL A 145       1.449  17.034  19.995  1.00 25.76 AAAA
ATOM   1049  N   MET A 146       0.324  15.208  19.289  1.00 26.18 AAAA
ATOM   1050  CA  MET A 146       1.421  14.654  18.503  1.00 26.41 AAAA
ATOM   1051  CB  MET A 146       2.000  13.396  19.172  1.00 26.85 AAAA
ATOM   1052  CG  MET A 146       2.826  13.653  20.430  1.00 25.85 AAAA
ATOM   1053  SD  MET A 146       3.306  12.116  21.269  1.00 28.45 AAAA
ATOM   1054  CE  MET A 146       1.827  11.741  22.217  1.00 26.47 AAAA
ATOM   1055  C   MET A 146       0.860  14.293  17.131  1.00 27.20 AAAA
ATOM   1056  O   MET A 146      -0.311  13.934  16.998  1.00 25.68 AAAA
ATOM   1057  N   GLN A 147       1.701  14.395  16.111  1.00 28.03 AAAA
ATOM   1058  CA  GLN A 147       1.294  14.091  14.748  1.00 28.39 AAAA
ATOM   1059  CB  GLN A 147       1.067  15.388  13.979  1.00 28.65 AAAA
ATOM   1060  CG  GLN A 147       2.203  16.371  14.142  1.00 30.13 AAAA
ATOM   1061  CD  GLN A 147       2.006  17.653  13.360  1.00 29.84 AAAA
ATOM   1062  OE1 GLN A 147       2.730  18.629  13.565  1.00 32.18 AAAA
ATOM   1063  NE2 GLN A 147       1.036  17.657  12.453  1.00 29.40 AAAA
ATOM   1064  C   GLN A 147       2.394  13.274  14.085  1.00 29.45 AAAA
ATOM   1065  O   GLN A 147       3.570  13.420  14.424  1.00 29.21 AAAA
ATOM   1066  N   ALA A 148       2.010  12.412  13.150  1.00 29.90 AAAA
ATOM   1067  CA  ALA A 148       2.975  11.563  12.461  1.00 31.39 AAAA
ATOM   1068  CB  ALA A 148       2.254  10.468  11.690  1.00 30.97 AAAA
ATOM   1069  C   ALA A 148       3.846  12.373  11.514  1.00 32.66 AAAA
ATOM   1070  O   ALA A 148       5.071  12.231  11.517  1.00 32.76 AAAA
ATOM   1071  N   PHE A 149       3.205  13.220  10.712  1.00 33.44 AAAA
ATOM   1072  CA  PHE A 149       3.903  14.059   9.744  1.00 35.09 AAAA
ATOM   1073  CB  PHE A 149       3.367  13.814   8.332  1.00 34.59 AAAA
ATOM   1074  CG  PHE A 149       3.200  12.367   7.985  1.00 35.35 AAAA
ATOM   1075  CD1 PHE A 149       1.935  11.789   7.958  1.00 34.17 AAAA
ATOM   1076  CD2 PHE A 149       4.304  11.579   7.685  1.00 34.88 AAAA
ATOM   1077  CE1 PHE A 149       1.771  10.448   7.637  1.00 34.20 AAAA
ATOM   1078  CE2 PHE A 149       4.148  10.236   7.364  1.00 36.09 AAAA
ATOM   1079  CZ  PHE A 149       2.878   9.670   7.340  1.00 35.09 AAAA
ATOM   1080  C   PHE A 149       3.719  15.536  10.056  1.00 36.17 AAAA
ATOM   1081  O   PHE A 149       2.697  15.939  10.606  1.00 37.06 AAAA
ATOM   1082  N   PRO A 150       4.709  16.370   9.704  1.00 37.23 AAAA
ATOM   1083  CD  PRO A 150       6.002  16.078   9.056  1.00 37.75 AAAA
ATOM   1084  CA  PRO A 150       4.569  17.803   9.975  1.00 38.03 AAAA
ATOM   1085  CB  PRO A 150       5.967  18.341   9.682  1.00 38.69 AAAA
ATOM   1086  CG  PRO A 150       6.432  17.448   8.569  1.00 38.52 AAAA
ATOM   1087  C   PRO A 150       3.510  18.369   9.028  1.00 38.18 AAAA
ATOM   1088  O   PRO A 150       3.355  17.878   7.912  1.00 38.42 AAAA
ATOM   1089  N   GLY A 151       2.763  19.374   9.475  1.00 38.74 AAAA
ATOM   1090  CA  GLY A 151       1.749  19.952   8.609  1.00 38.66 AAAA
ATOM   1091  C   GLY A 151       0.300  19.705   8.996  1.00 38.69 AAAA
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ATOM   1092  O   GLY A 151      -0.571  20.502   8.645  1.00 38.08 AAAA
ATOM   1093  N   ALA A 152       0.024  18.602   9.689  1.00 38.70 AAAA
ATOM   1094  CA  ALA A 152      -1.343  18.311  10.112  1.00 38.90 AAAA
ATOM   1095  CB  ALA A 152      -1.402  16.980  10.859  1.00 38.46 AAAA
ATOM   1096  C   ALA A 152      -1.729  19.461  11.032  1.00 39.30 AAAA
ATOM   1097  O   ALA A 152      -2.753  20.114  10.838  1.00 40.05 AAAA
ATOM   1098  N   PHE A 153      -0.887  19.700  12.031  1.00 39.42 AAAA
ATOM   1099  CA  PHE A 153      -1.084  20.795  12.971  1.00 39.90 AAAA
ATOM   1100  CB  PHE A 153      -1.209  20.286  14.409  1.00 39.04 AAAA
ATOM   1101  CG  PHE A 153      -2.478  19.535  14.685  1.00 38.06 AAAA
ATOM   1102  CD1 PHE A 153      -2.571  18.175  14.419  1.00 36.71 AAAA
ATOM   1103  CD2 PHE A 153      -3.582  20.190  15.228  1.00 37.52 AAAA
ATOM   1104  CE1 PHE A 153      -3.747  17.475  14.692  1.00 36.39 AAAA
ATOM   1105  CE2 PHE A 153      -4.761  19.500  15.502  1.00 36.08 AAAA
ATOM   1106  CZ  PHE A 153      -4.842  18.140  15.235  1.00 36.20 AAAA
ATOM   1107  C   PHE A 153       0.143  21.696  12.865  1.00 40.75 AAAA
ATOM   1108  O   PHE A 153       1.238  21.228  12.543  1.00 41.03 AAAA
ATOM   1109  N   PRO A 154      -0.026  23.001  13.128  1.00 41.05 AAAA
ATOM   1110  CD  PRO A 154      -1.328  23.667  13.304  1.00 41.17 AAAA
ATOM   1111  CA  PRO A 154       1.052  23.992  13.068  1.00 41.57 AAAA
ATOM   1112  CB  PRO A 154       0.339  25.292  13.428  1.00 41.69 AAAA
ATOM   1113  CG  PRO A 154      -1.024  25.081  12.876  1.00 41.76 AAAA
ATOM   1114  C   PRO A 154       2.260  23.744  13.975  1.00 42.12 AAAA
ATOM   1115  O   PRO A 154       3.400  23.833  13.515  1.00 43.15 AAAA
ATOM   1116  N   ASN A 155       2.023  23.432  15.249  1.00 41.75 AAAA
ATOM   1117  CA  ASN A 155       3.135  23.230  16.180  1.00 41.57 AAAA
ATOM   1118  CB  ASN A 155       3.180  24.389  17.179  1.00 44.02 AAAA
ATOM   1119  CG  ASN A 155       2.961  25.736  16.522  1.00 45.69 AAAA
ATOM   1120  OD1 ASN A 155       1.862  26.045  16.058  1.00 47.64 AAAA
ATOM   1121  ND2 ASN A 155       4.010  26.545  16.475  1.00 47.43 AAAA
ATOM   1122  C   ASN A 155       3.193  21.921  16.970  1.00 40.83 AAAA
ATOM   1123  O   ASN A 155       3.973  21.814  17.917  1.00 41.17 AAAA
ATOM   1124  N   ALA A 156       2.390  20.929  16.601  1.00 38.83 AAAA
ATOM   1125  CA  ALA A 156       2.400  19.658  17.326  1.00 37.19 AAAA
ATOM   1126  CB  ALA A 156       1.203  18.811  16.909  1.00 36.03 AAAA
ATOM   1127  C   ALA A 156       3.698  18.882  17.090  1.00 35.95 AAAA
ATOM   1128  O   ALA A 156       4.206  18.834  15.971  1.00 35.55 AAAA
ATOM   1129  N   GLU A 157       4.233  18.275  18.146  1.00 35.08 AAAA
ATOM   1130  CA  GLU A 157       5.464  17.505  18.022  1.00 33.77 AAAA
ATOM   1131  CB  GLU A 157       5.848  16.881  19.373  1.00 34.33 AAAA
ATOM   1132  CG  GLU A 157       7.175  16.124  19.352  1.00 34.59 AAAA
ATOM   1133  CD  GLU A 157       7.487  15.430  20.670  1.00 35.45 AAAA
ATOM   1134  OE1 GLU A 157       8.517  14.729  20.746  1.00 34.09 AAAA
ATOM   1135  OE2 GLU A 157       6.705  15.582  21.631  1.00 36.21 AAAA
ATOM   1136  C   GLU A 157       5.282  16.405  16.970  1.00 32.70 AAAA
ATOM   1137  O   GLU A 157       4.262  15.709  16.952  1.00 31.88 AAAA
ATOM   1138  N   VAL A 158       6.268  16.265  16.088  1.00 31.00 AAAA
ATOM   1139  CA  VAL A 158       6.230  15.255  15.032  1.00 30.25 AAAA
ATOM   1140  CB  VAL A 158       6.926  15.768  13.751  1.00 30.33 AAAA
ATOM   1141  CG1 VAL A 158       7.013  14.653  12.719  1.00 29.98 AAAA
ATOM   1142  CG2 VAL A 158       6.147  16.953  13.181  1.00 30.15 AAAA
ATOM   1143  C   VAL A 158       6.937  13.998  15.529  1.00 29.69 AAAA
ATOM   1144  O   VAL A 158       8.142  14.020  15.798  1.00 29.80 AAAA
ATOM   1145  N   VAL A 159       6.182  12.909  15.645  1.00 28.61 AAAA
ATOM   1146  CA  VAL A 159       6.715  11.647  16.149  1.00 29.00 AAAA
ATOM   1147  CB  VAL A 159       6.019  11.250  17.469  1.00 28.75 AAAA
ATOM   1148  CG1 VAL A 159       6.129  12.384  18.482  1.00 28.06 AAAA
ATOM   1149  CG2 VAL A 159       4.552  10.921  17.197  1.00 28.06 AAAA
ATOM   1150  C   VAL A 159       6.581  10.469  15.186  1.00 29.32 AAAA
ATOM   1151  O   VAL A 159       7.066   9.376  15.479  1.00 29.89 AAAA
ATOM   1152  N   GLY A 160       5.915  10.688  14.054  1.00 30.03 AAAA
ATOM   1153  CA  GLY A 160       5.727   9.628  13.075  1.00 29.63 AAAA
ATOM   1154  C   GLY A 160       4.678   8.608  13.483  1.00 29.61 AAAA
ATOM   1155  O   GLY A 160       3.917   8.849  14.416  1.00 29.30 AAAA
ATOM   1156  N   ASN A 161       4.635   7.475  12.782  1.00 29.30 AAAA
ATOM   1157  CA  ASN A 161       3.677   6.401  13.074  1.00 29.78 AAAA
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ATOM   1158  CB  ASN A 161       2.800   6.097  11.858  1.00 30.70 AAAA
ATOM   1159  CG  ASN A 161       1.755   7.154  11.609  1.00 32.16 AAAA
ATOM   1160  OD1 ASN A 161       0.951   7.461  12.492  1.00 31.78 AAAA
ATOM   1161  ND2 ASN A 161       1.750   7.711  10.400  1.00 30.88 AAAA
ATOM   1162  C   ASN A 161       4.344   5.089  13.462  1.00 29.50 AAAA
ATOM   1163  O   ASN A 161       5.471   4.810  13.058  1.00 29.61 AAAA
ATOM   1164  N   PRO A 162       3.648   4.263  14.251  1.00 29.59 AAAA
ATOM   1165  CD  PRO A 162       2.441   4.571  15.039  1.00 29.95 AAAA
ATOM   1166  CA  PRO A 162       4.219   2.977  14.650  1.00 29.65 AAAA
ATOM   1167  CB  PRO A 162       3.143   2.389  15.553  1.00 29.79 AAAA
ATOM   1168  CG  PRO A 162       2.559   3.608  16.200  1.00 30.38 AAAA
ATOM   1169  C   PRO A 162       4.423   2.135  13.389  1.00 30.13 AAAA
ATOM   1170  O   PRO A 162       3.535   2.063  12.531  1.00 28.48 AAAA
ATOM   1171  N   VAL A 163       5.590   1.508  13.287  1.00 29.92 AAAA
ATOM   1172  CA  VAL A 163       5.935   0.664  12.149  1.00 29.89 AAAA
ATOM   1173  CB  VAL A 163       7.182   1.224  11.417  1.00 31.04 AAAA
ATOM   1174  CG1 VAL A 163       7.571   0.308  10.260  1.00 30.44 AAAA
ATOM   1175  CG2 VAL A 163       6.902   2.631  10.914  1.00 29.10 AAAA
ATOM   1176  C   VAL A 163       6.258  -0.744  12.652  1.00 31.06 AAAA
ATOM   1177  O   VAL A 163       6.884  -0.892  13.706  1.00 29.66 AAAA
ATOM   1178  N   ARG A 164       5.820  -1.773  11.927  1.00 31.83 AAAA
ATOM   1179  CA  ARG A 164       6.124  -3.142  12.339  1.00 34.34 AAAA
ATOM   1180  CB  ARG A 164       5.533  -4.167  11.354  1.00 36.31 AAAA
ATOM   1181  CG  ARG A 164       5.704  -3.841   9.876  1.00 39.86 AAAA
ATOM   1182  CD  ARG A 164       4.855  -4.770   8.997  1.00 41.13 AAAA
ATOM   1183  NE  ARG A 164       5.368  -6.140   8.946  1.00 43.44 AAAA
ATOM   1184  CZ  ARG A 164       4.765  -7.145   8.311  1.00 44.08 AAAA
ATOM   1185  NH1 ARG A 164       3.619  -6.940   7.671  1.00 44.91 AAAA
ATOM   1186  NH2 ARG A 164       5.308  -8.355   8.308  1.00 44.44 AAAA
ATOM   1187  C   ARG A 164       7.649  -3.248  12.419  1.00 34.72 AAAA
ATOM   1188  O   ARG A 164       8.364  -2.769  11.537  1.00 33.63 AAAA
ATOM   1189  N   THR A 165       8.138  -3.855  13.496  1.00 34.72 AAAA
ATOM   1190  CA  THR A 165       9.567  -3.969  13.730  1.00 34.94 AAAA
ATOM   1191  CB  THR A 165       9.839  -4.437  15.177  1.00 35.90 AAAA
ATOM   1192  OG1 THR A 165       9.008  -5.563  15.488  1.00 36.96 AAAA
ATOM   1193  CG2 THR A 165       9.530  -3.313  16.149  1.00 35.88 AAAA
ATOM   1194  C   THR A 165      10.373  -4.814  12.749  1.00 34.61 AAAA
ATOM   1195  O   THR A 165      11.577  -4.603  12.608  1.00 34.56 AAAA
ATOM   1196  N   ASP A 166       9.739  -5.765  12.068  1.00 34.66 AAAA
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AAAAATOM	2325	CA	ALA	A	316	4.940	3.172	-17.250	1.00	34.17
AAAAATOM	2326	CB	ALA	A	316	4.469	2.616	-18.593	1.00	33.68
AAAAATOM	2327	C	ALA	A	316	6.002	4.252	-17.456	1.00	34.75
AAAAATOM	2328	O	ALA	A	316	7.190	4.026	-17.211	1.00	34.70
AAAAATOM	2329	N	ASN	A	317	5.578	5.434	-17.889	1.00	35.49
AAAAATOM	2330	CA	ASN	A	317	6.524	6.518	-18.108	1.00	35.27
AAAAATOM	2331	CB	ASN	A	317	5.815	7.738	-18.694	1.00	37.74
AAAAATOM	2332	CG	ASN	A	317	5.395	7.518	-20.128	1.00	38.86
AAAAATOM	2333	OD1	ASN	A	317	6.099	6.855	-20.889	1.00	39.80
AAAAATOM	2334	ND2	ASN	A	317	4.252	8.077	-20.511	1.00	40.96
AAAAATOM	2335	C	ASN	A	317	7.272	6.916	-16.847	1.00	35.18
AAAAATOM	2336	O	ASN	A	317	8.458	7.239	-16.904	1.00	34.36
AAAAATOM	2337	N	THR	A	318	6.592	6.891	-15.704	1.00	34.31
AAAAATOM	2338	CA	THR	A	318	7.251	7.262	-14.456	1.00	34.35
AAAAATOM	2339	CB	THR	A	318	6.245	7.358	-13.282	1.00	34.55
AAAAATOM	2340	OG1	THR	A	318	5.353	8.460	-13.498	1.00	34.46
AAAAATOM	2341	CG2	THR	A	318	6.984	7.568	-11.969	1.00	34.42
AAAAATOM	2342	C	THR	A	318	8.335	6.252	-14.093	1.00	34.52
AAAAATOM	2343	O	THR	A	318	9.464	6.624	-13.783	1.00	34.11
AAAAATOM	2344	N	LEU	A	319	7.987	4.971	-14.139	1.00	35.35
AAAAATOM	2345	CA	LEU	A	319	8.937	3.918	-13.801	1.00	35.23
AAAAATOM	2346	CB	LEU	A	319	8.233	2.556	-13.804	1.00	34.91
AAAAATOM	2347	CG	LEU	A	319	7.142	2.362	-12.743	1.00	34.50
AAAAATOM	2348	CD1	LEU	A	319	6.445	1.031	-12.956	1.00	34.48
AAAAATOM	2349	CD2	LEU	A	319	7.761	2.432	-11.351	1.00	35.13
AAAAATOM	2350	C	LEU	A	319	10.107	3.907	-14.777	1.00	35.72
AAAAATOM	2351	O	LEU	A	319	11.264	3.830	-14.370	1.00	34.85

AAAAATOM	2352	N	ALA	A	320	9.801	3.997	-16.067	1.00	36.49
AAAAATOM	2353	CA	ALA	A	320	10.832	3.989	-17.096	1.00	38.10
AAAAATOM	2354	CB	ALA	A	320	10.192	4.051	-18.472	1.00	37.58
AAAAATOM	2355	C	ALA	A	320	11.809	5.144	-16.924	1.00	38.94
AAAAATOM	2356	O	ALA	A	320	12.939	5.087	-17.410	1.00	39.51
AAAAATOM	2357	N	GLY	A	321	11.375	6.186	-16.219	1.00	38.88
AAAAATOM	2358	CA	GLY	A	321	12.224	7.347	-16.013	1.00	38.68
AAAAATOM	2359	C	GLY	A	321	13.117	7.303	-14.788	1.00	38.70
AAAAATOM	2360	O	GLY	A	321	13.881	8.235	-14.542	1.00	38.64
AAAAATOM	2361	N	TRP	A	322	13.028	6.230	-14.010	1.00	38.46
AAAAATOM	2362	CA	TRP	A	322	13.855	6.108	-12.820	1.00	38.53
AAAAATOM	2363	CB	TRP	A	322	13.008	5.688	-11.611	1.00	39.41
AAAAATOM	2364	CG	TRP	A	322	12.047	6.748	-11.146	1.00	40.01
AAAAATOM	2365	CD2	TRP	A	322	10.898	6.558	-10.307	1.00	40.49
AAAAATOM	2366	CE2	TRP	A	322	10.330	7.833	-10.081	1.00	41.27
AAAAATOM	2367	CE3	TRP	A	322	10.295	5.436	-9.722	1.00	40.54
AAAAATOM	2368	CD1	TRP	A	322	12.126	8.091	-11.389	1.00	39.97
AAAAATOM	2369	NE1	TRP	A	322	11.098	8.749	-10.752	1.00	40.69
AAAAATOM	2370	CZ2	TRP	A	322	9.186	8.018	-9.293	1.00	41.67
AAAAATOM	2371	CZ3	TRP	A	322	9.155	5.619	-8.938	1.00	41.40
AAAAATOM	2372	CH2	TRP	A	322	8.615	6.903	-8.732	1.00	41.69
AAAAATOM	2373	C	TRP	A	322	14.984	5.109	-13.027	1.00	38.48
AAAAATOM	2374	O	TRP	A	322	14.743	3.929	-13.271	1.00	38.22
AAAAATOM	2375	N	SER	A	323	16.217	5.596	-12.935	1.00	38.13
AAAAATOM	2376	CA	SER	A	323	17.395	4.753	-13.101	1.00	38.51
AAAAATOM	2377	CB	SER	A	323	18.573	5.590	-13.591	1.00	38.51
AAAAATOM	2378	OG	SER	A	323	18.994	6.489	-12.582	1.00	39.52
AAAAATOM	2379	C	SER	A	323	17.739	4.150	-11.744	1.00	38.37
AAAAATOM	2380	O	SER	A	323	17.188	4.566	-10.725	1.00	37.29
AAAAATOM	2381	N	ARG	A	324	18.647	3.178	-11.723	1.00	37.86
AAAAATOM	2382	CA	ARG	A	324	19.030	2.563	-10.461	1.00	37.82
AAAAATOM	2383	CB	ARG	A	324	19.924	1.341	-10.688	1.00	36.36
AAAAATOM	2384	CG	ARG	A	324	19.130	0.077	-10.959	1.00	34.77
AAAAATOM	2385	CD	ARG	A	324	19.978	-1.176	-10.849	1.00	33.04
AAAAATOM	2386	NE	ARG	A	324	19.143	-2.372	-10.888	1.00	31.23
AAAAATOM	2387	CZ	ARG	A	324	18.318	-2.738	-9.908	1.00	29.95
AAAAATOM	2388	NH1	ARG	A	324	18.228	-2.006	-8.808	1.00	28.46
AAAAATOM	2389	NH2	ARG	A	324	17.562	-3.815	-10.041	1.00	28.17
AAAAATOM	2390	C	ARG	A	324	19.731	3.571	-9.569	1.00	38.78
AAAAATOM	2391	O	ARG	A	324	19.532	3.578	-8.354	1.00	38.12
AAAAATOM	2392	N	GLU	A	325	20.551	4.428	-10.169	1.00	39.55
AAAAATOM	2393	CA	GLU	A	325	21.251	5.447	-9.401	1.00	40.60
AAAAATOM	2394	CB	GLU	A	325	22.208	6.236	-10.304	1.00	42.74
AAAAATOM	2395	CG	GLU	A	325	22.642	7.589	-9.745	1.00	46.19
AAAAATOM	2396	CD	GLU	A	325	23.197	7.517	-8.327	1.00	48.10
AAAAATOM	2397	OE1	GLU	A	325	23.535	8.586	-7.770	1.00	49.61
AAAAATOM	2398	OE2	GLU	A	325	23.297	6.403	-7.768	1.00	49.87
AAAAATOM	2399	C	GLU	A	325	20.214	6.380	-8.784	1.00	39.88
AAAAATOM	2400	O	GLU	A	325	20.324	6.771	-7.623	1.00	39.45
AAAAATOM	2401	N	THR	A	326	19.202	6.725	-9.572	1.00	39.89
AAAAATOM	2402	CA	THR	A	326	18.130	7.591	-9.102	1.00	40.25
AAAAATOM	2403	CB	THR	A	326	17.139	7.912	-10.240	1.00	40.72
AAAAATOM	2404	OG1	THR	A	326	17.828	8.593	-11.298	1.00	42.28
AAAAATOM	2405	CG2	THR	A	326	16.006	8.795	-9.730	1.00	41.64
AAAAATOM	2406	C	THR	A	326	17.371	6.897	-7.968	1.00	39.76
AAAAATOM	2407	O	THR	A	326	17.108	7.497	-6.925	1.00	39.87
AAAAATOM	2408	N	LEU	A	327	17.027	5.628	-8.175	1.00	38.46
AAAAATOM	2409	CA	LEU	A	327	16.294	4.867	-7.169	1.00	37.41
AAAAATOM	2410	CB	LEU	A	327	15.968	3.466	-7.697	1.00	36.19
AAAAATOM	2411	CG	LEU	A	327	14.952	3.426	-8.843	1.00	35.32
AAAAATOM	2412	CD1	LEU	A	327	14.802	2.002	-9.370	1.00	35.07
AAAAATOM	2413	CD2	LEU	A	327	13.614	3.961	-8.354	1.00	34.69
AAAAATOM	2414	C	LEU	A	327	17.050	4.774	-5.845	1.00	37.39
AAAAATOM	2415	O	LEU	A	327	16.437	4.807	-4.778	1.00	36.80
AAAAATOM	2416	N	LEU	A	328	18.375	4.665	-5.909	1.00	37.58
AAAAATOM	2417	CA	LEU	A	328	19.184	4.593	-4.693	1.00	38.35

AAAAATOM	2418	CB	LEU	A	328	20.662	4.368	-5.030	1.00	38.95
AAAAATOM	2419	CG	LEU	A	328	21.636	4.544	-3.854	1.00	40.10
AAAAATOM	2420	CD1	LEU	A	328	21.303	3.551	-2.752	1.00	39.51
AAAAATOM	2421	CD2	LEU	A	328	23.068	4.349	-4.330	1.00	40.30
AAAAATOM	2422	C	LEU	A	328	19.039	5.899	-3.926	1.00	38.68
AAAAATOM	2423	O	LEU	A	328	18.929	5.906	-2.697	1.00	38.65
AAAAATOM	2424	N	THR	A	329	19.048	7.004	-4.664	1.00	39.35
AAAAATOM	2425	CA	THR	A	329	18.908	8.326	-4.068	1.00	39.98
AAAAATOM	2426	CB	THR	A	329	19.002	9.433	-5.136	1.00	40.05
AAAAATOM	2427	OG1	THR	A	329	20.280	9.364	-5.782	1.00	41.54
AAAAATOM	2428	CG2	THR	A	329	18.841	10.808	-4.497	1.00	40.35
AAAAATOM	2429	C	THR	A	329	17.557	8.425	-3.367	1.00	39.68
AAAAATOM	2430	O	THR	A	329	17.485	8.743	-2.179	1.00	39.91
AAAAATOM	2431	N	MET	A	330	16.492	8.147	-4.111	1.00	39.51
AAAAATOM	2432	CA	MET	A	330	15.143	8.190	-3.564	1.00	38.79
AAAAATOM	2433	CB	MET	A	330	14.141	7.718	-4.617	1.00	38.09
AAAAATOM	2434	CG	MET	A	330	14.011	8.657	-5.804	1.00	36.84
AAAAATOM	2435	SD	MET	A	330	12.977	7.980	-7.108	1.00	37.95
AAAAATOM	2436	CE	MET	A	330	11.332	8.342	-6.478	1.00	37.58
AAAAATOM	2437	C	MET	A	330	15.037	7.315	-2.319	1.00	39.71
AAAAATOM	2438	O	MET	A	330	14.418	7.703	-1.326	1.00	39.60
AAAAATOM	2439	N	ALA	A	331	15.646	6.135	-2.381	1.00	39.50
AAAAATOM	2440	CA	ALA	A	331	15.625	5.202	-1.266	1.00	40.36
AAAAATOM	2441	CB	ALA	A	331	16.378	3.928	-1.634	1.00	39.91
AAAAATOM	2442	C	ALA	A	331	16.243	5.843	-0.032	1.00	40.98
AAAAATOM	2443	O	ALA	A	331	15.662	5.805	1.052	1.00	40.34
AAAAATOM	2444	N	GLU	A	332	17.422	6.435	-0.201	1.00	41.85
AAAAATOM	2445	CA	GLU	A	332	18.102	7.087	0.911	1.00	42.77
AAAAATOM	2446	CB	GLU	A	332	19.470	7.607	0.465	1.00	44.04
AAAAATOM	2447	CG	GLU	A	332	20.414	6.500	0.016	1.00	46.55
AAAAATOM	2448	CD	GLU	A	332	21.822	6.994	-0.248	1.00	48.04
AAAAATOM	2449	OE1	GLU	A	332	21.981	7.923	-1.065	1.00	49.87
AAAAATOM	2450	OE2	GLU	A	332	22.770	6.449	0.359	1.00	49.38
AAAAATOM	2451	C	GLU	A	332	17.246	8.228	1.445	1.00	42.38
AAAAATOM	2452	O	GLU	A	332	17.156	8.435	2.653	1.00	42.66
AAAAATOM	2453	N	ARG	A	333	16.619	8.969	0.540	1.00	41.80
AAAAATOM	2454	CA	ARG	A	333	15.752	10.067	0.937	1.00	42.25
AAAAATOM	2455	CB	ARG	A	333	15.212	10.784	-0.306	1.00	43.43
AAAAATOM	2456	CG	ARG	A	333	16.184	11.793	-0.926	1.00	45.99
AAAAATOM	2457	CD	ARG	A	333	15.844	12.060	-2.389	1.00	48.51
AAAAATOM	2458	NE	ARG	A	333	16.415	13.301	-2.913	1.00	50.45
AAAAATOM	2459	CZ	ARG	A	333	17.703	13.631	-2.859	1.00	52.07
AAAAATOM	2460	NH1	ARG	A	333	18.585	12.814	-2.297	1.00	52.45
AAAAATOM	2461	NH2	ARG	A	333	18.112	14.784	-3.377	1.00	51.94
AAAAATOM	2462	C	ARG	A	333	14.594	9.519	1.777	1.00	41.39
AAAAATOM	2463	O	ARG	A	333	14.275	10.060	2.834	1.00	40.21
AAAAATOM	2464	N	ALA	A	334	13.981	8.435	1.308	1.00	40.03
AAAAATOM	2465	CA	ALA	A	334	12.859	7.825	2.014	1.00	39.84
AAAAATOM	2466	CB	ALA	A	334	12.356	6.612	1.241	1.00	38.43
AAAAATOM	2467	C	ALA	A	334	13.239	7.417	3.435	1.00	40.05
AAAAATOM	2468	O	ALA	A	334	12.493	7.665	4.386	1.00	40.41
AAAAATOM	2469	N	ARG	A	335	14.404	6.797	3.577	1.00	39.11
AAAAATOM	2470	CA	ARG	A	335	14.874	6.351	4.881	1.00	40.00
AAAAATOM	2471	CB	ARG	A	335	16.137	5.506	4.719	1.00	39.98
AAAAATOM	2472	CG	ARG	A	335	16.631	4.865	6.000	1.00	40.54
AAAAATOM	2473	CD	ARG	A	335	15.653	3.814	6.501	1.00	42.08
AAAAATOM	2474	NE	ARG	A	335	16.263	2.949	7.507	1.00	42.95
AAAAATOM	2475	CZ	ARG	A	335	16.403	1.634	7.373	1.00	43.43
AAAAATOM	2476	NH1	ARG	A	335	15.972	1.024	6.274	1.00	43.17
AAAAATOM	2477	NH2	ARG	A	335	16.983	0.927	8.335	1.00	43.96
AAAAATOM	2478	C	ARG	A	335	15.167	7.527	5.802	1.00	40.09
AAAAATOM	2479	O	ARG	A	335	14.877	7.479	6.997	1.00	39.35
AAAAATOM	2480	N	ALA	A	336	15.745	8.581	5.237	1.00	40.52
AAAAATOM	2481	CA	ALA	A	336	16.089	9.774	6.001	1.00	41.50
AAAAATOM	2482	CB	ALA	A	336	16.850	10.754	5.116	1.00	41.05
AAAAATOM	2483	C	ALA	A	336	14.847	10.447	6.573	1.00	42.00

AAAAATOM	2484	O	ALA	A	336	14.905	11.087	7.621	1.00	42.49
AAAAATOM	2485	N	ALA	A	337	13.725	10.300	5.879	1.00	42.58
AAAAATOM	2486	CA	ALA	A	337	12.475	10.903	6.320	1.00	42.55
AAAAATOM	2487	CB	ALA	A	337	11.656	11.338	5.111	1.00	42.34
AAAAATOM	2488	C	ALA	A	337	11.670	9.932	7.174	1.00	42.43
AAAAATOM	2489	O	ALA	A	337	10.444	10.000	7.209	1.00	44.01
AAAAATOM	2490	N	SER	A	338	12.360	9.035	7.868	1.00	41.93
AAAAATOM	2491	CA	SER	A	338	11.686	8.053	8.708	1.00	41.12
AAAAATOM	2492	CB	SER	A	338	12.097	6.641	8.293	1.00	40.73
AAAAATOM	2493	OG	SER	A	338	11.504	5.671	9.139	1.00	40.32
AAAAATOM	2494	C	SER	A	338	11.964	8.235	10.198	1.00	40.88
AAAAATOM	2495	O	SER	A	338	13.042	8.674	10.594	1.00	41.46
AAAAATOM	2496	N	ILE	A	339	10.971	7.898	11.013	1.00	40.11
AAAAATOM	2497	CA	ILE	A	339	11.080	7.985	12.461	1.00	39.66
AAAAATOM	2498	CB	ILE	A	339	10.061	8.992	13.038	1.00	39.74
AAAAATOM	2499	CG2	ILE	A	339	10.249	9.118	14.544	1.00	38.88
AAAAATOM	2500	CG1	ILE	A	339	10.249	10.354	12.361	1.00	39.75
AAAAATOM	2501	CD1	ILE	A	339	9.263	11.423	12.804	1.00	40.42
AAAAATOM	2502	C	ILE	A	339	10.788	6.576	12.978	1.00	40.19
AAAAATOM	2503	O	ILE	A	339	9.653	6.102	12.923	1.00	39.97
AAAAATOM	2504	N	PRO	A	340	11.821	5.886	13.484	1.00	40.75
AAAAATOM	2505	CD	PRO	A	340	13.225	6.336	13.448	1.00	40.95
AAAAATOM	2506	CA	PRO	A	340	11.728	4.520	14.012	1.00	40.57
AAAAATOM	2507	CB	PRO	A	340	13.161	4.021	13.877	1.00	41.22
AAAAATOM	2508	CG	PRO	A	340	13.944	5.244	14.222	1.00	41.12
AAAAATOM	2509	C	PRO	A	340	11.180	4.294	15.424	1.00	40.38
AAAAATOM	2510	O	PRO	A	340	10.841	3.163	15.776	1.00	40.48
AAAAATOM	2511	N	ASP	A	341	11.080	5.345	16.232	1.00	39.43
AAAAATOM	2512	CA	ASP	A	341	10.603	5.174	17.603	1.00	38.32
AAAAATOM	2513	CB	ASP	A	341	11.668	5.696	18.578	1.00	38.62
AAAAATOM	2514	CG	ASP	A	341	12.044	7.146	18.317	1.00	39.54
AAAAATOM	2515	OD1	ASP	A	341	11.727	7.658	17.221	1.00	38.30
AAAAATOM	2516	OD2	ASP	A	341	12.668	7.771	19.209	1.00	40.07
AAAAATOM	2517	C	ASP	A	341	9.241	5.789	17.939	1.00	37.27
AAAAATOM	2518	O	ASP	A	341	9.014	6.235	19.066	1.00	35.88
AAAAATOM	2519	N	ALA	A	342	8.329	5.789	16.971	1.00	36.20
AAAAATOM	2520	CA	ALA	A	342	6.996	6.349	17.181	1.00	34.98
AAAAATOM	2521	CB	ALA	A	342	6.150	6.156	15.927	1.00	35.84
AAAAATOM	2522	C	ALA	A	342	6.280	5.744	18.389	1.00	34.17
AAAAATOM	2523	O	ALA	A	342	5.843	6.465	19.289	1.00	33.36
AAAAATOM	2524	N	THR	A	343	6.159	4.421	18.410	1.00	33.49
AAAAATOM	2525	CA	THR	A	343	5.481	3.747	19.512	1.00	33.39
AAAAATOM	2526	CB	THR	A	343	5.567	2.211	19.362	1.00	33.34
AAAAATOM	2527	OG1	THR	A	343	4.951	1.818	18.128	1.00	34.05
AAAAATOM	2528	CG2	THR	A	343	4.851	1.519	20.516	1.00	33.82
AAAAATOM	2529	C	THR	A	343	6.067	4.155	20.865	1.00	33.89
AAAAATOM	2530	O	THR	A	343	5.340	4.591	21.756	1.00	32.15
AAAAATOM	2531	N	GLU	A	344	7.383	4.027	21.007	1.00	34.87
AAAAATOM	2532	CA	GLU	A	344	8.055	4.379	22.257	1.00	35.80
AAAAATOM	2533	CB	GLU	A	344	9.553	4.054	22.177	1.00	37.79
AAAAATOM	2534	CG	GLU	A	344	9.892	2.570	22.029	1.00	41.45
AAAAATOM	2535	CD	GLU	A	344	9.963	2.101	20.581	1.00	44.16
AAAAATOM	2536	OE1	GLU	A	344	10.311	0.917	20.357	1.00	45.57
AAAAATOM	2537	OE2	GLU	A	344	9.676	2.910	19.668	1.00	45.28
AAAAATOM	2538	C	GLU	A	344	7.886	5.856	22.590	1.00	35.95
AAAAATOM	2539	O	GLU	A	344	7.751	6.233	23.754	1.00	35.12
AAAAATOM	2540	N	ARG	A	345	7.896	6.689	21.559	1.00	35.83
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BBBBATOM   2754  O   PRO B  22       2.129 -39.522 -33.321  1.00 24.40
BBBBATOM   2755  N   GLY B  23       1.585 -41.102 -31.807  1.00 24.71
BBBBATOM   2756  CA  GLY B  23       0.787 -41.864 -32.752  1.00 25.07
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BBBBATOM   2775  CG1 VAL B  26       1.410 -40.833 -38.479  1.00 26.25
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BBBBATOM   2784  N   HIS B  28      -3.864 -37.933 -36.847  1.00 27.68
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BBBBATOM   2791  NE2 HIS B  28      -6.578 -36.417 -33.101  1.00 27.78
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BBBBATOM   2973  O   LEU B  50     -8.769 -40.477 -26.882  1.00 32.52
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BBBBATOM   2975  CA  VAL B  51     -8.299 -42.641 -28.449  1.00 32.68
BBBBATOM   2976  CB  VAL B  51     -7.829 -43.982 -29.058  1.00 33.06
BBBBATOM   2977  CG1 VAL B  51     -8.115 -44.013 -30.565  1.00 31.54
BBBBATOM   2978  CG2 VAL B  51     -6.329 -44.145 -28.813  1.00 31.45
BBBBATOM   2979  C   VAL B  51     -9.747 -42.348 -28.829  1.00 33.08
BBBBATOM   2980  O   VAL B  51    -10.000 -41.623 -29.792  1.00 32.88
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BBBBATOM   2982  CD  PRO B  52    -10.667 -44.012 -27.119  1.00 33.29
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BBBBATOM   2985  CG  PRO B  52    -12.021 -44.661 -27.307  1.00 33.77
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BBBBATOM   3001  CD2 HIS B  54     -7.360 -37.760 -28.406  1.00 33.76
BBBBATOM   3002  ND1 HIS B  54     -6.884 -36.869 -30.343  1.00 34.27
BBBBATOM   3003  CE1 HIS B  54     -6.120 -36.277 -29.441  1.00 34.41
BBBBATOM   3004  NE2 HIS B  54     -6.390 -36.799 -28.258  1.00 33.91
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BBBBATOM   3014  CG2 ILE B  56     -8.761 -43.602 -34.245  1.00 32.87
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BBBBATOM   3026  C   GLU B  57    -11.044 -46.923 -33.005  1.00 33.01
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BBBBATOM   3040  OD1 ASP B  59    -11.969 -53.037 -33.812  1.00 32.40
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BBBBATOM   3043  O   ASP B  59     -7.987 -52.491 -30.492  1.00 30.24
BBBBATOM   3044  N   PHE B  60     -9.608 -53.888 -29.815  1.00 30.65
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BBBBATOM   3109  C    ARG B  67       5.071 -58.142 -20.713  1.00 29.99
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BBBBATOM   3118  CG   LYS B  69       6.757 -62.360 -21.794  1.00 25.08
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BBBBATOM   3120  CE   LYS B  69       5.357 -64.358 -21.035  1.00 28.31
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BBBBATOM   3128  N    ILE B  71      10.819 -61.373 -27.814  1.00 21.85
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BBBBATOM   3153  CG  LEU B  74       6.422 -62.208 -26.884  1.00 18.80
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BBBBATOM   3157  O   LEU B  74       5.539 -66.779 -26.863  1.00 20.01
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BBBBATOM   3177  CD  PRO B  78       4.211 -71.603 -25.976  1.00 21.89
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BBBBATOM   3194  CG  ARG B  80      -1.286 -67.051 -23.118  1.00 24.03
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BBBBATOM   3198  NH1 ARG B  80      1.290 -66.349 -19.787  1.00 26.92
BBBBATOM   3199  NH2 ARG B  80      2.514 -68.152 -20.519  1.00 27.22
BBBBATOM   3200  C   ARG B  80     -0.526 -66.233 -26.790  1.00 21.29
BBBBATOM   3201  O   ARG B  80     -1.278 -65.355 -27.223  1.00 21.47
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BBBBATOM   3203  CA  ILE B  81      1.113 -65.621 -28.421  1.00 19.47
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BBBBATOM   3208  C   ILE B  81      0.256 -65.937 -29.654  1.00 18.99
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BBBBATOM	3402	CE1	TYR	B	106	6.043	-53.915	-22.108	1.00	33.13
BBBBATOM	3403	CD2	TYR	B	106	6.058	-55.631	-24.282	1.00	31.27
BBBBATOM	3404	CE2	TYR	B	106	7.234	-55.400	-23.569	1.00	32.27
BBBBATOM	3405	CZ	TYR	B	106	7.219	-54.541	-22.487	1.00	33.19
BBBBATOM	3406	OH	TYR	B	106	8.388	-54.291	-21.802	1.00	35.95
BBBBATOM	3407	C	TYR	B	106	2.719	-55.018	-27.100	1.00	20.52
BBBBATOM	3408	O	TYR	B	106	2.867	-56.052	-27.746	1.00	20.50
BBBBATOM	3409	N	VAL	B	107	1.628	-54.270	-27.205	1.00	19.06
BBBBATOM	3410	CA	VAL	B	107	0.557	-54.694	-28.099	1.00	18.06
BBBBATOM	3411	CB	VAL	B	107	-0.690	-53.774	-27.978	1.00	20.95
BBBBATOM	3412	CG1	VAL	B	107	-0.407	-52.407	-28.589	1.00	21.39
BBBBATOM	3413	CG2	VAL	B	107	-1.879	-54.433	-28.658	1.00	21.30
BBBBATOM	3414	C	VAL	B	107	1.015	-54.743	-29.559	1.00	17.45
BBBBATOM	3415	O	VAL	B	107	0.502	-55.536	-30.346	1.00	16.99
BBBBATOM	3416	N	SER	B	108	1.991	-53.916	-29.918	1.00	17.96
BBBBATOM	3417	CA	SER	B	108	2.488	-53.892	-31.290	1.00	19.67
BBBBATOM	3418	CB	SER	B	108	3.424	-52.691	-31.508	1.00	19.56
BBBBATOM	3419	OG	SER	B	108	4.666	-52.824	-30.837	1.00	19.63
BBBBATOM	3420	C	SER	B	108	3.197	-55.187	-31.694	1.00	20.38
BBBBATOM	3421	O	SER	B	108	3.385	-55.449	-32.884	1.00	21.25
BBBBATOM	3422	N	GLY	B	109	3.595	-55.995	-30.710	1.00	19.59
BBBBATOM	3423	CA	GLY	B	109	4.251	-57.256	-31.023	1.00	20.03
BBBBATOM	3424	C	GLY	B	109	3.311	-58.170	-31.792	1.00	19.61
BBBBATOM	3425	O	GLY	B	109	3.579	-58.517	-32.940	1.00	19.24
BBBBATOM	3426	N	PRO	B	110	2.206	-58.606	-31.173	1.00	19.20
BBBBATOM	3427	CD	PRO	B	110	1.914	-58.528	-29.729	1.00	19.94
BBBBATOM	3428	CA	PRO	B	110	1.251	-59.478	-31.855	1.00	18.99
BBBBATOM	3429	CB	PRO	B	110	0.198	-59.737	-30.778	1.00	20.41
BBBBATOM	3430	CG	PRO	B	110	0.998	-59.720	-29.515	1.00	19.81
BBBBATOM	3431	C	PRO	B	110	0.651	-58.761	-33.075	1.00	19.22
BBBBATOM	3432	O	PRO	B	110	0.406	-59.371	-34.116	1.00	17.13
BBBBATOM	3433	N	GLY	B	111	0.407	-57.462	-32.927	1.00	19.03
BBBBATOM	3434	CA	GLY	B	111	-0.160	-56.702	-34.025	1.00	19.60
BBBBATOM	3435	C	GLY	B	111	0.764	-56.714	-35.226	1.00	19.59
BBBBATOM	3436	O	GLY	B	111	0.330	-56.979	-36.339	1.00	21.10
BBBBATOM	3437	N	GLY	B	112	2.043	-56.429	-34.995	1.00	19.78
BBBBATOM	3438	CA	GLY	B	112	3.014	-56.417	-36.074	1.00	19.97
BBBBATOM	3439	C	GLY	B	112	3.147	-57.783	-36.724	1.00	20.43
BBBBATOM	3440	O	GLY	B	112	3.233	-57.896	-37.949	1.00	19.94
BBBBATOM	3441	N	LEU	B	113	3.167	-58.828	-35.903	1.00	19.26
BBBBATOM	3442	CA	LEU	B	113	3.265	-60.184	-36.429	1.00	19.49
BBBBATOM	3443	CB	LEU	B	113	3.405	-61.198	-35.289	1.00	18.38
BBBBATOM	3444	CG	LEU	B	113	4.777	-61.270	-34.605	1.00	20.59
BBBBATOM	3445	CD1	LEU	B	113	4.656	-62.059	-33.311	1.00	20.01
BBBBATOM	3446	CD2	LEU	B	113	5.794	-61.914	-35.538	1.00	20.23
BBBBATOM	3447	C	LEU	B	113	2.040	-60.521	-37.274	1.00	18.73
BBBBATOM	3448	O	LEU	B	113	2.143	-61.252	-38.255	1.00	18.44
BBBBATOM	3449	N	ALA	B	114	0.875	-60.010	-36.892	1.00	18.96
BBBBATOM	3450	CA	ALA	B	114	-0.334	-60.292	-37.661	1.00	18.70
BBBBATOM	3451	CB	ALA	B	114	-1.562	-59.855	-36.889	1.00	16.45
BBBBATOM	3452	C	ALA	B	114	-0.288	-59.578	-39.019	1.00	19.30
BBBBATOM	3453	O	ALA	B	114	-0.602	-60.167	-40.052	1.00	20.62
BBBBATOM	3454	N	ALA	B	115	0.082	-58.303	-39.000	1.00	20.57
BBBBATOM	3455	CA	ALA	B	115	0.167	-57.516	-40.229	1.00	21.84
BBBBATOM	3456	CB	ALA	B	115	0.636	-56.108	-39.911	1.00	19.85
BBBBATOM	3457	C	ALA	B	115	1.140	-58.192	-41.189	1.00	21.58
BBBBATOM	3458	O	ALA	B	115	0.815	-58.464	-42.345	1.00	22.14

BBBBATOM	3459	N	TRP	B	116	2.334	-58.476	-40.688	1.00 22.12
BBBBATOM	3460	CA	TRP	B	116	3.365	-59.526	-41.478	1.00 23.22
BBBBATOM	3461	CB	TRP	B	116	4.584	-59.367	-40.579	1.00 26.08
BBBBATOM	3462	CG	TRP	B	116	5.699	-60.136	-41.204	1.00 27.40
BBBBATOM	3463	CD2	TRP	B	116	6.168	-61.418	-40.793	1.00 28.77
BBBBATOM	3464	CE2	TRP	B	116	7.234	-61.771	-41.655	1.00 30.37
BBBBATOM	3465	CE3	TRP	B	116	5.794	-62.308	-39.778	1.00 30.49
BBBBATOM	3466	CD1	TRP	B	116	6.473	-59.761	-42.271	1.00 28.30
BBBBATOM	3467	NE1	TRP	B	116	7.401	-60.742	-42.547	1.00 29.04
BBBBATOM	3468	CZ2	TRP	B	116	7.929	-62.981	-41.529	1.00 31.08
BBBBATOM	3469	CZ3	TRP	B	116	6.485	-63.510	-39.653	1.00 31.85
BBBBATOM	3470	CH2	TRP	B	116	7.541	-63.834	-40.527	1.00 32.27
BBBBATOM	3471	C	TRP	B	116	2.871	-60.434	-42.123	1.00 23.55
BBBBATOM	3472	O	TRP	B	116	3.048	-60.643	-43.329	1.00 22.19
BBBBATOM	3473	N	SER	B	117	2.231	-61.304	-41.338	1.00 21.35
BBBBATOM	3474	CA	SER	B	117	1.735	-62.573	-41.873	1.00 22.61
BBBBATOM	3475	CB	SER	B	117	1.167	-63.462	-40.756	1.00 20.72
BBBBATOM	3476	OG	SER	B	117	0.010	-62.889	-40.169	1.00 22.72
BBBBATOM	3477	C	SER	B	117	0.665	-62.383	-42.940	1.00 23.56
BBBBATOM	3478	O	SER	B	117	0.463	-63.262	-43.780	1.00 23.11
BBBBATOM	3479	N	LEU	B	118	-0.020	-61.242	-42.905	1.00 24.40
BBBBATOM	3480	CA	LEU	B	118	-1.069	-60.957	-43.882	1.00 25.70
BBBBATOM	3481	CB	LEU	B	118	-2.195	-60.155	-43.227	1.00 25.80
BBBBATOM	3482	CG	LEU	B	118	-3.012	-60.889	-42.159	1.00 26.56
BBBBATOM	3483	CD1	LEU	B	118	-3.905	-59.895	-41.433	1.00 26.62
BBBBATOM	3484	CD2	LEU	B	118	-3.841	-62.000	-42.801	1.00 26.51
BBBBATOM	3485	C	LEU	B	118	-0.539	-60.193	-45.094	1.00 26.87
BBBBATOM	3486	O	LEU	B	118	-1.292	-59.878	-46.021	1.00 26.69
BBBBATOM	3487	N	GLY	B	119	0.755	-59.898	-45.085	1.00 26.39
BBBBATOM	3488	CA	GLY	B	119	1.354	-59.174	-46.192	1.00 27.80
BBBBATOM	3489	C	GLY	B	119	1.142	-57.671	-46.120	1.00 27.64
BBBBATOM	3490	O	GLY	B	119	1.293	-56.972	-47.122	1.00 28.49
BBBBATOM	3491	N	ILE	B	120	0.786	-57.173	-44.940	1.00 25.88
BBBBATOM	3492	CA	ILE	B	120	0.568	-55.744	-44.731	1.00 24.85
BBBBATOM	3493	CB	ILE	B	120	-0.507	-55.497	-43.652	1.00 24.64
BBBBATOM	3494	CG2	ILE	B	120	-0.648	-54.000	-43.397	1.00 24.49
BBBBATOM	3495	CG1	ILE	B	120	-1.839	-56.112	-44.093	1.00 24.61
BBBBATOM	3496	CD1	ILE	B	120	-2.891	-56.170	-42.991	1.00 23.34
BBBBATOM	3497	C	ILE	B	120	1.879	-55.121	-44.272	1.00 24.55
BBBBATOM	3498	O	ILE	B	120	2.465	-55.551	-43.275	1.00 23.69
BBBBATOM	3499	N	PRO	B	121	2.365	-54.098	-44.995	1.00 23.85
BBBBATOM	3500	CD	PRO	B	121	1.780	-53.400	-46.154	1.00 23.64
BBBBATOM	3501	CA	PRO	B	121	3.625	-53.477	-44.591	1.00 22.63
BBBBATOM	3502	CB	PRO	B	121	3.872	-52.440	-45.691	1.00 23.83
BBBBATOM	3503	CG	PRO	B	121	2.485	-52.053	-46.102	1.00 23.96
BBBBATOM	3504	C	PRO	B	121	3.583	-52.869	-43.196	1.00 22.21
BBBBATOM	3505	O	PRO	B	121	2.617	-52.208	-42.810	1.00 22.46
BBBBATOM	3506	N	VAL	B	122	4.641	-53.114	-42.437	1.00 21.69
BBBBATOM	3507	CA	VAL	B	122	4.743	-52.594	-41.083	1.00 22.03
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BBBBATOM	3510	CG2	VAL	B	122	4.133	-54.789	-40.035	1.00 22.19
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BBBBATOM	3513	N	VAL	B	123	5.330	-50.338	-40.464	1.00 20.94
BBBBATOM	3514	CA	VAL	B	123	6.200	-49.184	-40.310	1.00 20.82
BBBBATOM	3515	CB	VAL	B	123	5.580	-47.902	-40.932	1.00 22.16
BBBBATOM	3516	CG1	VAL	B	123	6.516	-46.722	-40.709	1.00 20.83
BBBBATOM	3517	CG2	VAL	B	123	5.322	-48.111	-42.420	1.00 22.66
BBBBATOM	3518	C	VAL	B	123	6.338	-48.953	-38.812	1.00 21.09
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BBBBATOM	3520	N	LEU	B	124	7.557	-48.720	-38.340	1.00 20.53
BBBBATOM	3521	CA	LEU	B	124	7.749	-48.485	-36.915	1.00 22.10
BBBBATOM	3522	CB	LEU	B	124	8.578	-49.606	-36.286	1.00 22.00
BBBBATOM	3523	CG	LEU	B	124	8.160	-51.051	-36.551	1.00 22.45
BBBBATOM	3524	CD1	LEU	B	124	9.196	-51.974	-35.905	1.00 23.90

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BBBBATOM   3525  CD2 LEU B 124      6.765 -51.313 -36.003  1.00 22.34
BBBBATOM   3526  C   LEU B 124      8.452 -47.472 -36.633  1.00 22.36
BBBBATOM   3527  O   LEU B 124      9.218 -46.660 -37.461  1.00 20.75
BBBBATOM   3528  N   HIS B 125      8.182 -46.638 -35.447  1.00 21.40
BBBBATOM   3529  CA  HIS B 125      8.814 -45.413 -34.981  1.00 21.42
BBBBATOM   3530  CB  HIS B 125      7.858 -44.218 -35.067  1.00 21.57
BBBBATOM   3531  CG  HIS B 125      8.432 -42.948 -34.511  1.00 23.73
BBBBATOM   3532  CD2 HIS B 125      8.300 -42.368 -33.295  1.00 22.15
BBBBATOM   3533  ND1 HIS B 125      9.274 -42.127 -35.236  1.00 26.23
BBBBATOM   3534  CE1 HIS B 125      9.631 -41.095 -34.490  1.00 24.20
BBBBATOM   3535  NE2 HIS B 125      9.054 -41.218 -33.307  1.00 26.07
BBBBATOM   3536  C   HIS B 125      9.196 -45.642 -33.519  1.00 21.70
BBBBATOM   3537  O   HIS B 125      8.378 -46.117 -32.725  1.00 19.81
BBBBATOM   3538  N   GLU B 126     10.444 -45.332 -33.186  1.00 21.20
BBBBATOM   3539  CA  GLU B 126     10.947 -45.452 -31.817  1.00 22.15
BBBBATOM   3540  CB  GLU B 126     12.252 -46.246 -31.790  1.00 21.99
BBBBATOM   3541  CG  GLU B 126     12.958 -46.206 -30.439  1.00 22.04
BBBBATOM   3542  CD  GLU B 126     12.119 -46.824 -29.338  1.00 21.43
BBBBATOM   3543  OE1 GLU B 126     11.767 -48.014 -29.471  1.00 21.92
BBBBATOM   3544  OE2 GLU B 126     11.807 -46.124 -28.349  1.00 21.08
BBBBATOM   3545  C   GLU B 126     11.205 -44.027 -31.326  1.00 21.93
BBBBATOM   3546  O   GLU B 126     12.016 -43.300 -31.908  1.00 21.33
BBBBATOM   3547  N   GLN B 127     10.520 -43.624 -30.259  1.00 22.62
BBBBATOM   3548  CA  GLN B 127     10.682 -42.270 -29.735  1.00 22.81
BBBBATOM   3549  CB  GLN B 127      9.414 -41.814 -28.989  1.00 23.56
BBBBATOM   3550  CG  GLN B 127      8.147 -41.783 -29.830  1.00 24.46
BBBBATOM   3551  CD  GLN B 127      7.312 -43.041 -29.687  1.00 25.85
BBBBATOM   3552  OE1 GLN B 127      6.842 -43.366 -28.591  1.00 23.78
BBBBATOM   3553  NE2 GLN B 127      7.119 -43.758 -30.797  1.00 24.91
BBBBATOM   3554  C   GLN B 127     11.874 -42.087 -28.809  1.00 22.39
BBBBATOM   3555  O   GLN B 127     12.399 -40.976 -28.682  1.00 22.43
BBBBATOM   3556  N   ASN B 128     12.314 -43.173 -28.177  1.00 22.35
BBBBATOM   3557  CA  ASN B 128     13.406 -43.097 -27.216  1.00 22.96
BBBBATOM   3558  CB  ASN B 128     13.136 -44.080 -26.064  1.00 22.85
BBBBATOM   3559  CG  ASN B 128     11.742 -43.919 -25.474  1.00 23.25
BBBBATOM   3560  OD1 ASN B 128     10.804 -44.632 -25.848  1.00 26.04
BBBBATOM   3561  ND2 ASN B 128     11.597 -42.975 -24.556  1.00 22.68
BBBBATOM   3562  C   ASN B 128     14.824 -43.314 -27.742  1.00 23.87
BBBBATOM   3563  O   ASN B 128     15.026 -43.856 -28.830  1.00 24.05
BBBBATOM   3564  N   GLY B 129     15.798 -42.885 -26.940  1.00 24.35
BBBBATOM   3565  CA  GLY B 129     17.203 -43.019 -27.294  1.00 25.36
BBBBATOM   3566  C   GLY B 129     17.642 -44.468 -27.280  1.00 25.97
BBBBATOM   3567  O   GLY B 129     18.643 -44.836 -27.891  1.00 25.48
BBBBATOM   3568  N   ILE B 130     16.886 -45.290 -26.565  1.00 26.18
BBBBATOM   3569  CA  ILE B 130     17.160 -46.716 -26.488  1.00 28.00
BBBBATOM   3570  CB  ILE B 130     17.480 -47.145 -25.033  1.00 28.45
BBBBATOM   3571  CG2 ILE B 130     16.323 -46.785 -24.102  1.00 28.52
BBBBATOM   3572  CG1 ILE B 130     17.776 -48.642 -24.986  1.00 29.33
BBBBATOM   3573  CD1 ILE B 130     18.097 -49.149 -23.593  1.00 31.39
BBBBATOM   3574  C   ILE B 130     15.909 -47.435 -26.999  1.00 27.44
BBBBATOM   3575  O   ILE B 130     14.793 -47.103 -26.610  1.00 28.58
BBBBATOM   3576  N   ALA B 131     16.097 -48.405 -27.887  1.00 26.98
BBBBATOM   3577  CA  ALA B 131     14.978 -49.139 -28.461  1.00 25.88
BBBBATOM   3578  CB  ALA B 131     15.485 -50.102 -29.525  1.00 25.02
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BBBBATOM   3581  N   GLY B 132     12.851 -49.814 -27.506  1.00 24.52
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BBBBATOM   3583  C   GLY B 132     12.150 -52.019 -26.831  1.00 23.35
BBBBATOM   3584  O   GLY B 132     12.582 -52.419 -27.904  1.00 22.89
BBBBATOM   3585  N   LEU B 133     11.788 -52.846 -25.860  1.00 23.38
BBBBATOM   3586  CA  LEU B 133     11.903 -54.293 -26.020  1.00 24.54
BBBBATOM   3587  CB  LEU B 133     11.328 -54.996 -24.786  1.00 25.48
BBBBATOM   3588  CG  LEU B 133     11.388 -56.527 -24.780  1.00 27.50
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BBBBATOM   3593  N    THR B 134       9.975 -54.401 -27.499  1.00 21.72
BBBBATOM   3594  CA   THR B 134       9.202 -54.860 -28.639  1.00 21.22
BBBBATOM   3595  CB   THR B 134       7.716 -54.509 -28.449  1.00 20.99
BBBBATOM   3596  OG1  THR B 134       7.257 -55.075 -27.210  1.00 20.94
BBBBATOM   3597  CG2  THR B 134       6.872 -55.073 -29.600  1.00 20.64
BBBBATOM   3598  C    THR B 134       9.693 -54.326 -29.986  1.00 20.62
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BBBBATOM   3600  N    ASN B 135       9.932 -53.021 -30.075  1.00 21.24
BBBBATOM   3601  CA   ASN B 135      10.407 -52.419 -31.324  1.00 20.50
BBBBATOM   3602  CB   ASN B 135      10.637 -50.911 -31.142  1.00 19.58
BBBBATOM   3603  CG   ASN B 135       9.457 -50.058 -31.597  1.00 19.93
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BBBBATOM   3606  C    ASN B 135      11.724 -53.064 -31.767  1.00 20.78
BBBBATOM   3607  O    ASN B 135      11.945 -53.290 -32.953  1.00 20.41
BBBBATOM   3608  N    LYS B 136      12.595 -53.366 -30.809  1.00 21.46
BBBBATOM   3609  CA   LYS B 136      13.886 -53.949 -31.144  1.00 22.79
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BBBBATOM   3618  CA   TRP B 137      12.753 -57.345 -32.424  1.00 22.06
BBBBATOM   3619  CB   TRP B 137      12.361 -58.552 -31.553  1.00 21.20
BBBBATOM   3620  CG   TRP B 137      10.990 -58.525 -30.922  1.00 20.23
BBBBATOM   3621  CD2  TRP B 137       9.748 -58.877 -31.544  1.00 18.68
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BBBBATOM   3626  CZ2  TRP B 137       7.401 -59.058 -30.821  1.00 18.18
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BBBBATOM   3632  CA   LEU B 138       9.744 -56.188 -34.431  1.00 23.15
BBBBATOM   3633  CB   LEU B 138       8.618 -55.305 -33.886  1.00 23.87
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BBBBATOM   3635  CD1  LEU B 138       6.672 -56.508 -34.915  1.00 25.34
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BBBBATOM   3639  N    ALA B 139      11.423 -54.763 -35.453  1.00 23.34
BBBBATOM   3640  CA   ALA B 139      12.128 -54.092 -36.542  1.00 25.29
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BBBBATOM   3642  C    ALA B 139      12.624 -55.064 -37.610  1.00 26.83
BBBBATOM   3643  O    ALA B 139      12.829 -54.672 -38.754  1.00 27.29
BBBBATOM   3644  N    LYS B 140      12.801 -56.332 -37.241  1.00 27.38
BBBBATOM   3645  CA   LYS B 140      13.279 -57.337 -38.182  1.00 28.05
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BBBBATOM   3647  CG   LYS B 140      15.134 -58.057 -36.635  1.00 31.62
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BBBBATOM   3654  CA   ILE B 141       9.963 -57.818 -40.016  1.00 26.09
BBBBATOM   3655  CB   ILE B 141       8.854 -58.721 -39.405  1.00 26.39
BBBBATOM   3656  CG2  ILE B 141       9.401 -60.118 -39.145  1.00 28.33
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BBBBATOM   3676  CG  LYS B 144     10.202 -46.710 -43.013  1.00 27.44
BBBBATOM   3677  CD  LYS B 144     11.602 -46.480 -43.558  1.00 29.01
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BBBBATOM   3679  NZ  LYS B 144     13.406 -44.774 -43.854  1.00 31.29
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BBBBATOM   3684  CB  VAL B 145     12.981 -49.279 -38.617  1.00 23.66
BBBBATOM   3685  CG1 VAL B 145     13.083 -49.014 -37.114  1.00 24.44
BBBBATOM   3686  CG2 VAL B 145     12.589 -50.724 -38.878  1.00 23.51
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BBBBATOM   3688  O   VAL B 145     13.473 -46.545 -39.808  1.00 23.68
BBBBATOM   3689  N   MET B 146     11.902 -46.103 -38.251  1.00 23.84
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BBBBATOM   3691  CB  MET B 146     11.274 -43.729 -38.448  1.00 24.72
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BBBBATOM   3696  O   MET B 146     11.963 -45.311 -35.689  1.00 22.43
BBBBATOM   3697  N   GLN B 147     13.456 -43.678 -36.112  1.00 23.37
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BBBBATOM   3702  OE1 GLN B 147     18.425 -44.671 -35.637  1.00 28.62
BBBBATOM   3703  NE2 GLN B 147     17.615 -44.966 -33.558  1.00 26.05
BBBBATOM   3704  C   GLN B 147     13.880 -41.911 -34.515  1.00 26.28
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BBBBATOM   3820  CB  ARG B 164       3.430 -28.411 -28.833  1.00 34.56
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BBBBATOM   3823  NE  ARG B 164       2.481 -27.555 -26.299  1.00 44.08
BBBBATOM   3824  CZ  ARG B 164       2.307 -26.919 -25.144  1.00 45.79
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BBBBATOM   3849  C   VAL B 167       7.548 -24.361 -30.736  1.00 25.54
BBBBATOM   3850  O   VAL B 167       8.548 -23.642 -30.787  1.00 25.58
BBBBATOM   3851  N   LEU B 168       7.108 -25.059 -31.778  1.00 26.75
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BBBBATOM   3854  CG  LEU B 168       7.205 -27.440 -33.890  1.00 28.67
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BBBBATOM   3887  N   PRO B 173     16.735 -18.959 -31.190  1.00 25.73
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BBBBATOM   3906  CG  GLN B 175     14.206 -12.805 -32.888  1.00 33.70
BBBBATOM   3907  CD  GLN B 175     13.324 -13.006 -34.109  1.00 35.20
BBBBATOM   3908  OE1 GLN B 175     12.247 -12.422 -34.215  1.00 38.98
BBBBATOM   3909  NE2 GLN B 175     13.785 -13.828 -35.042  1.00 37.92
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BBBBATOM   3919  NH1 ARG B 176     15.121 -19.233 -26.107  1.00 41.22
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BBBBATOM   4050  N    ARG B 196       9.195 -34.592  -7.426  1.00 32.81
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BBBBATOM	4074	CD2	LEU	B	198	14.692	-31.146	-10.493	1.00	25.94
BBBBATOM	4075	C	LEU	B	198	12.388	-29.893	-7.006	1.00	26.41
BBBBATOM	4076	O	LEU	B	198	12.930	-28.835	-6.667	1.00	26.35
BBBBATOM	4077	N	ASN	B	199	11.205	-30.274	-6.532	1.00	26.01
BBBBATOM	4078	CA	ASN	B	199	10.497	-29.447	-5.563	1.00	27.07
BBBBATOM	4079	CB	ASN	B	199	9.123	-30.035	-5.238	1.00	26.63
BBBBATOM	4080	CG	ASN	B	199	8.212	-30.050	-6.434	1.00	27.62
BBBBATOM	4081	OD1	ASN	B	199	8.519	-29.434	-7.460	1.00	26.33
BBBBATOM	4082	ND2	ASN	B	199	7.080	-30.749	-6.320	1.00	24.20
BBBBATOM	4083	C	ASN	B	199	11.308	-29.319	-4.282	1.00	27.65
BBBBATOM	4084	O	ASN	B	199	11.207	-28.321	-3.581	1.00	28.19
BBBBATOM	4085	N	GLN	B	200	12.124	-30.328	-3.994	1.00	28.38
BBBBATOM	4086	CA	GLN	B	200	12.955	-30.326	-2.794	1.00	30.10
BBBBATOM	4087	CB	GLN	B	200	13.158	-31.764	-2.301	1.00	31.91
BBBBATOM	4088	CG	GLN	B	200	11.883	-32.453	-1.827	1.00	35.02
BBBBATOM	4089	CD	GLN	B	200	12.056	-33.956	-1.632	1.00	37.49
BBBBATOM	4090	OE1	GLN	B	200	11.204	-34.619	-1.032	1.00	38.76
BBBBATOM	4091	NE2	GLN	B	200	13.155	-34.502	-2.151	1.00	37.28
BBBBATOM	4092	C	GLN	B	200	14.319	-29.675	-3.011	1.00	30.18
BBBBATOM	4093	O	GLN	B	200	14.834	-28.975	-2.135	1.00	31.13
BBBBATOM	4094	N	THR	B	201	14.897	-29.884	-4.187	1.00	28.94
BBBBATOM	4095	CA	THR	B	201	16.215	-29.345	-4.474	1.00	27.34
BBBBATOM	4096	CB	THR	B	201	16.915	-30.181	-5.567	1.00	28.81
BBBBATOM	4097	OG1	THR	B	201	16.988	-31.553	-5.149	1.00	28.92
BBBBATOM	4098	CG2	THR	B	201	18.331	-29.654	-5.817	1.00	28.29
BBBBATOM	4099	C	THR	B	201	16.313	-27.871	-4.869	1.00	25.78
BBBBATOM	4100	O	THR	B	201	17.137	-27.138	-4.331	1.00	24.91
BBBBATOM	4101	N	MET	B	202	15.479	-27.430	-5.800	1.00	24.08
BBBBATOM	4102	CA	MET	B	202	15.567	-26.048	-6.268	1.00	23.68
BBBBATOM	4103	CB	MET	B	202	14.558	-25.827	-7.397	1.00	22.29
BBBBATOM	4104	CG	MET	B	202	14.856	-26.685	-8.633	1.00	22.80
BBBBATOM	4105	SD	MET	B	202	16.590	-26.614	-9.190	1.00	25.93
BBBBATOM	4106	CE	MET	B	202	16.814	-24.877	-9.345	1.00	22.63
BBBBATOM	4107	C	MET	B	202	15.489	-24.926	-5.229	1.00	23.47
BBBBATOM	4108	O	MET	B	202	16.189	-23.929	-5.354	1.00	24.40
BBBBATOM	4109	N	PRO	B	203	14.636	-25.059	-4.192	1.00	24.12
BBBBATOM	4110	CD	PRO	B	203	13.518	-25.991	-3.970	1.00	22.27
BBBBATOM	4111	CA	PRO	B	203	14.608	-23.963	-3.220	1.00	23.84
BBBBATOM	4112	CB	PRO	B	203	13.553	-24.424	-2.217	1.00	24.46
BBBBATOM	4113	CG	PRO	B	203	12.593	-25.178	-3.084	1.00	24.04
BBBBATOM	4114	C	PRO	B	203	15.987	-23.731	-2.573	1.00	24.07
BBBBATOM	4115	O	PRO	B	203	16.395	-22.593	-2.343	1.00	23.18
BBBBATOM	4116	N	GLN	B	204	16.706	-24.814	-2.290	1.00	25.26
BBBBATOM	4117	CA	GLN	B	204	18.033	-24.708	-1.684	1.00	26.34
BBBBATOM	4118	CB	GLN	B	204	18.474	-26.078	-1.157	1.00	28.67

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BBBBATOM   4119  CG  GLN B 204      17.555 -26.626  -0.065  1.00 33.65
BBBBATOM   4120  CD  GLN B 204      17.885 -28.059   0.328  1.00 37.09
BBBBATOM   4121  OE1 GLN B 204      18.991 -28.354   0.792  1.00 39.30
BBBBATOM   4122  NE2 GLN B 204      16.924 -28.960   0.140  1.00 38.32
BBBBATOM   4123  C   GLN B 204      19.030 -24.177  -2.717  1.00 25.36
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BBBBATOM   4125  N   VAL B 205      18.806 -24.522  -3.978  1.00 24.46
BBBBATOM   4126  CA  VAL B 205      19.672 -24.033  -5.043  1.00 24.44
BBBBATOM   4127  CB  VAL B 205      19.288 -24.634  -6.409  1.00 24.84
BBBBATOM   4128  CG1 VAL B 205      20.039 -23.906  -7.534  1.00 23.72
BBBBATOM   4129  CG2 VAL B 205      19.614 -26.110  -6.428  1.00 22.91
BBBBATOM   4130  C   VAL B 205      19.511 -22.515  -5.110  1.00 23.79
BBBBATOM   4131  O   VAL B 205      20.487 -21.789  -5.270  1.00 25.25
BBBBATOM   4132  N   ALA B 206      18.273 -22.044  -4.972  1.00 24.12
BBBBATOM   4133  CA  ALA B 206      17.980 -20.610  -5.013  1.00 22.84
BBBBATOM   4134  CB  ALA B 206      16.466 -20.377  -4.908  1.00 21.55
BBBBATOM   4135  C   ALA B 206      18.700 -19.862  -3.890  1.00 24.09
BBBBATOM   4136  O   ALA B 206      19.174 -18.740  -4.081  1.00 24.90
BBBBATOM   4137  N   ALA B 207      18.768 -20.477  -2.713  1.00 25.15
BBBBATOM   4138  CA  ALA B 207      19.442 -19.857  -1.576  1.00 26.65
BBBBATOM   4139  CB  ALA B 207      19.260 -20.710  -0.324  1.00 27.83
BBBBATOM   4140  C   ALA B 207      20.924 -19.686  -1.879  1.00 26.96
BBBBATOM   4141  O   ALA B 207      21.537 -18.693  -1.493  1.00 27.82
BBBBATOM   4142  N   LYS B 208      21.498 -20.651  -2.586  1.00 27.19
BBBBATOM   4143  CA  LYS B 208      22.915 -20.595  -2.919  1.00 28.31
BBBBATOM   4144  CB  LYS B 208      23.432 -21.989  -3.300  1.00 29.85
BBBBATOM   4145  CG  LYS B 208      23.030 -23.088  -2.329  1.00 32.97
BBBBATOM   4146  CD  LYS B 208      23.264 -22.667  -0.886  1.00 35.74
BBBBATOM   4147  CE  LYS B 208      22.689 -23.689   0.084  1.00 37.28
BBBBATOM   4148  NZ  LYS B 208      21.227 -23.899  -0.135  1.00 35.29
BBBBATOM   4149  C   LYS B 208      23.237 -19.624  -4.050  1.00 27.83
BBBBATOM   4150  O   LYS B 208      24.286 -18.978  -4.033  1.00 27.46
BBBBATOM   4151  N   LEU B 209      22.341 -19.517  -5.028  1.00 26.04
BBBBATOM   4152  CA  LEU B 209      22.577 -18.640  -6.171  1.00 25.68
BBBBATOM   4153  CB  LEU B 209      21.975 -19.268  -7.435  1.00 25.08
BBBBATOM   4154  CG  LEU B 209      22.534 -20.638  -7.844  1.00 25.01
BBBBATOM   4155  CD1 LEU B 209      21.797 -21.151  -9.074  1.00 25.67
BBBBATOM   4156  CD2 LEU B 209      24.029 -20.528  -8.119  1.00 25.13
BBBBATOM   4157  C   LEU B 209      22.075 -17.200  -6.007  1.00 25.59
BBBBATOM   4158  O   LEU B 209      22.496 -16.313  -6.742  1.00 25.26
BBBBATOM   4159  N   GLY B 210      21.185 -16.970  -5.045  1.00 26.27
BBBBATOM   4160  CA  GLY B 210      20.675 -15.628  -4.804  1.00 26.56
BBBBATOM   4161  C   GLY B 210      20.238 -14.836  -6.030  1.00 27.75
BBBBATOM   4162  O   GLY B 210      19.518 -15.349  -6.889  1.00 27.68
BBBBATOM   4163  N   ASP B 211      20.696 -13.585  -6.105  1.00 27.93
BBBBATOM   4164  CA  ASP B 211      20.370 -12.647  -7.190  1.00 28.28
BBBBATOM   4165  CB  ASP B 211      21.011 -11.283  -6.906  1.00 29.89
BBBBATOM   4166  CG  ASP B 211      20.351 -10.545  -5.768  1.00 31.43
BBBBATOM   4167  OD1 ASP B 211      20.864  -9.469  -5.398  1.00 32.43
BBBBATOM   4168  OD2 ASP B 211      19.323 -11.025  -5.249  1.00 33.41
BBBBATOM   4169  C   ASP B 211      20.768 -13.035  -8.615  1.00 27.77
BBBBATOM   4170  O   ASP B 211      20.320 -12.397  -9.578  1.00 26.32
BBBBATOM   4171  N   SER B 212      21.616 -14.048  -8.753  1.00 25.75
BBBBATOM   4172  CA  SER B 212      22.098 -14.474 -10.067  1.00 25.73
BBBBATOM   4173  CB  SER B 212      23.331 -15.376  -9.904  1.00 26.63
BBBBATOM   4174  OG  SER B 212      22.971 -16.596  -9.282  1.00 26.71
BBBBATOM   4175  C   SER B 212      21.062 -15.185 -10.943  1.00 23.61
BBBBATOM   4176  O   SER B 212      21.262 -15.334 -12.147  1.00 22.28
BBBBATOM   4177  N   VAL B 213      19.969 -15.644 -10.344  1.00 23.16
BBBBATOM   4178  CA  VAL B 213      18.925 -16.308 -11.116  1.00 20.76
BBBBATOM   4179  CB  VAL B 213      18.952 -17.867 -10.989  1.00 21.69
BBBBATOM   4180  CG1 VAL B 213      20.318 -18.423 -11.375  1.00 19.84
BBBBATOM   4181  CG2 VAL B 213      18.564 -18.288  -9.576  1.00 20.36
BBBBATOM   4182  C   VAL B 213      17.535 -15.871 -10.677  1.00 21.41
BBBBATOM   4183  O   VAL B 213      17.328 -15.396  -9.554  1.00 20.58
BBBBATOM   4184  N   THR B 214      16.593 -16.021 -11.595  1.00 19.82
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BBBBATOM   4186  CB  THR B 214      14.718 -14.478 -12.126  1.00 21.35
BBBBATOM   4187  OG1 THR B 214      13.323 -14.273 -11.870  1.00 21.93
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BBBBATOM   4191  N   ILE B 215      13.706 -17.569 -10.921  1.00 19.21
BBBBATOM   4192  CA  ILE B 215      13.076 -18.850 -11.169  1.00 18.75
BBBBATOM   4193  CB  ILE B 215      13.417 -19.828 -10.008  1.00 18.82
BBBBATOM   4194  CG2 ILE B 215      12.690 -21.157 -10.194  1.00 19.53
BBBBATOM   4195  CG1 ILE B 215      14.934 -20.030  -9.931  1.00 19.76
BBBBATOM   4196  CD1 ILE B 215      15.421 -20.656  -8.600  1.00 19.40
BBBBATOM   4197  C   ILE B 215      11.568 -18.837 -11.315  1.00 19.26
BBBBATOM   4198  O   ILE B 215      10.874 -18.025 -10.699  1.00 18.28
BBBBATOM   4199  N   TRP B 216      11.089 -19.737 -12.167  1.00 18.93
BBBBATOM   4200  CA  TRP B 216       9.661 -19.973 -12.378  1.00 19.34
BBBBATOM   4201  CB  TRP B 216       9.222 -19.631 -13.797  1.00 18.97
BBBBATOM   4202  CG  TRP B 216       7.757 -19.897 -14.065  1.00 20.09
BBBBATOM   4203  CD2 TRP B 216       7.015 -19.467 -15.211  1.00 19.61
BBBBATOM   4204  CE2 TRP B 216       5.705 -19.988 -15.085  1.00 19.98
BBBBATOM   4205  CE3 TRP B 216       7.329 -18.690 -16.333  1.00 19.39
BBBBATOM   4206  CD1 TRP B 216       6.888 -20.639 -13.303  1.00 19.30
BBBBATOM   4207  NE1 TRP B 216       5.653 -20.700 -13.914  1.00 20.95
BBBBATOM   4208  CZ2 TRP B 216       4.713 -19.759 -16.043  1.00 22.06
BBBBATOM   4209  CZ3 TRP B 216       6.336 -18.459 -17.288  1.00 20.42
BBBBATOM   4210  CH2 TRP B 216       5.047 -18.993 -17.134  1.00 21.16
BBBBATOM   4211  C   TRP B 216       9.629 -21.479 -12.176  1.00 19.95
BBBBATOM   4212  O   TRP B 216      10.114 -22.241 -13.010  1.00 19.91
BBBBATOM   4213  N   HIS B 217       9.067 -21.897 -11.050  1.00 21.62
BBBBATOM   4214  CA  HIS B 217       9.015 -23.303 -10.680  1.00 21.06
BBBBATOM   4215  CB  HIS B 217       9.553 -23.419  -9.242  1.00 20.56
BBBBATOM   4216  CG  HIS B 217       9.717 -24.824  -8.747  1.00 21.95
BBBBATOM   4217  CD2 HIS B 217       8.915 -25.910  -8.846  1.00 22.12
BBBBATOM   4218  ND1 HIS B 217      10.807 -25.219  -8.002  1.00 23.39
BBBBATOM   4219  CE1 HIS B 217      10.670 -26.490  -7.663  1.00 21.82
BBBBATOM   4220  NE2 HIS B 217       9.530 -26.933  -8.162  1.00 22.14
BBBBATOM   4221  C   HIS B 217       7.596 -23.870 -10.795  1.00 21.27
BBBBATOM   4222  O   HIS B 217       6.655 -23.334 -10.214  1.00 21.69
BBBBATOM   4223  N   GLN B 218       7.448 -24.940 -11.567  1.00 20.83
BBBBATOM   4224  CA  GLN B 218       6.149 -25.594 -11.735  1.00 24.30
BBBBATOM   4225  CB  GLN B 218       5.915 -25.935 -13.206  1.00 23.84
BBBBATOM   4226  CG  GLN B 218       4.561 -26.558 -13.495  1.00 25.91
BBBBATOM   4227  CD  GLN B 218       4.637 -28.060 -13.673  1.00 26.52
BBBBATOM   4228  OE1 GLN B 218       3.757 -28.793 -13.214  1.00 28.05
BBBBATOM   4229  NE2 GLN B 218       5.680 -28.529 -14.360  1.00 25.20
BBBBATOM   4230  C   GLN B 218       6.173 -26.854 -10.854  1.00 24.64
BBBBATOM   4231  O   GLN B 218       6.780 -27.866 -11.199  1.00 25.73
BBBBATOM   4232  N   SER B 219       5.502 -26.756  -9.709  1.00 26.38
BBBBATOM   4233  CA  SER B 219       5.463 -27.800  -8.684  1.00 26.73
BBBBATOM   4234  CB  SER B 219       4.947 -27.188  -7.380  1.00 28.26
BBBBATOM   4235  OG  SER B 219       3.563 -26.881  -7.488  1.00 26.22
BBBBATOM   4236  C   SER B 219       4.689 -29.096  -8.914  1.00 27.58
BBBBATOM   4237  O   SER B 219       5.014 -30.122  -8.320  1.00 26.39
BBBBATOM   4238  N   GLY B 220       3.662 -29.054  -9.750  1.00 28.58
BBBBATOM   4239  CA  GLY B 220       2.855 -30.242  -9.961  1.00 30.53
BBBBATOM   4240  C   GLY B 220       1.596 -30.110  -9.111  1.00 31.96
BBBBATOM   4241  O   GLY B 220       1.523 -29.248  -8.233  1.00 30.92
BBBBATOM   4242  N   LYS B 221       0.608 -30.965  -9.358  1.00 33.93
BBBBATOM   4243  CA  LYS B 221      -0.657 -30.914  -8.628  1.00 35.12
BBBBATOM   4244  CB  LYS B 221      -1.573 -32.049  -9.094  1.00 37.88
BBBBATOM   4245  CG  LYS B 221      -2.942 -32.055  -8.427  1.00 40.51
BBBBATOM   4246  CD  LYS B 221      -3.792 -33.215  -8.934  1.00 42.62
BBBBATOM   4247  CE  LYS B 221      -5.162 -33.249  -8.260  1.00 43.67
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BBBBATOM   4251  N   GLY B 222   -1.187 -29.979  -6.461  1.00 34.79
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BBBBATOM   4258  OG  SER B 223    3.303 -31.168  -4.897  1.00 36.07
BBBBATOM   4259  C   SER B 223    2.839 -27.454  -4.504  1.00 33.55
BBBBATOM   4260  O   SER B 223    3.930 -27.063  -4.086  1.00 31.72
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BBBBATOM   4262  CA  GLN B 224    2.187 -25.208  -5.186  1.00 33.71
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BBBBATOM   4265  CD  GLN B 224    1.344 -22.076  -5.249  1.00 40.08
BBBBATOM   4266  OE1 GLN B 224    0.669 -22.111  -4.217  1.00 40.97
BBBBATOM   4267  NE2 GLN B 224    2.244 -21.124  -5.486  1.00 40.08
BBBBATOM   4268  C   GLN B 224    2.510 -24.560  -3.840  1.00 33.86
BBBBATOM   4269  O   GLN B 224    3.512 -23.856  -3.697  1.00 33.38
BBBBATOM   4270  N   GLN B 225    1.659 -24.814  -2.850  1.00 33.06
BBBBATOM   4271  CA  GLN B 225    1.823 -24.239  -1.519  1.00 32.32
BBBBATOM   4272  CB  GLN B 225    0.624 -24.619  -0.640  1.00 35.12
BBBBATOM   4273  CG  GLN B 225   -0.743 -24.143  -1.151  1.00 36.85
BBBBATOM   4274  CD  GLN B 225   -1.144 -24.751  -2.495  1.00 39.09
BBBBATOM   4275  OE1 GLN B 225   -0.914 -25.937  -2.759  1.00 39.42
BBBBATOM   4276  NE2 GLN B 225   -1.768 -23.937  -3.345  1.00 40.13
BBBBATOM   4277  C   GLN B 225    3.117 -24.606  -0.788  1.00 30.73
BBBBATOM   4278  O   GLN B 225    3.766 -23.742  -0.202  1.00 30.36
BBBBATOM   4279  N   SER B 226    3.494 -25.878  -0.817  1.00 29.26
BBBBATOM   4280  CA  SER B 226    4.701 -26.309  -0.122  1.00 28.30
BBBBATOM   4281  CB  SER B 226    4.727 -27.834   0.003  1.00 29.10
BBBBATOM   4282  OG  SER B 226    4.563 -28.461  -1.254  1.00 32.61
BBBBATOM   4283  C   SER B 226    5.991 -25.809  -0.771  1.00 26.41
BBBBATOM   4284  O   SER B 226    6.950 -25.486  -0.073  1.00 25.24
BBBBATOM   4285  N   VAL B 227    6.019 -25.738  -2.099  1.00 25.21
BBBBATOM   4286  CA  VAL B 227    7.214 -25.247  -2.791  1.00 24.28
BBBBATOM   4287  CB  VAL B 227    7.150 -25.527  -4.317  1.00 23.32
BBBBATOM   4288  CG1 VAL B 227    8.368 -24.914  -5.028  1.00 20.67
BBBBATOM   4289  CG2 VAL B 227    7.117 -27.024  -4.563  1.00 22.45
BBBBATOM   4290  C   VAL B 227    7.335 -23.743  -2.545  1.00 24.34
BBBBATOM   4291  O   VAL B 227    8.421 -23.240  -2.281  1.00 25.50
BBBBATOM   4292  N   GLU B 228    6.209 -23.035  -2.623  1.00 26.12
BBBBATOM   4293  CA  GLU B 228    6.178 -21.592  -2.387  1.00 27.23
BBBBATOM   4294  CB  GLU B 228    4.735 -21.075  -2.476  1.00 28.60
BBBBATOM   4295  CG  GLU B 228    4.558 -19.586  -2.184  1.00 30.24
BBBBATOM   4296  CD  GLU B 228    4.938 -18.688  -3.356  1.00 31.99
BBBBATOM   4297  OE1 GLU B 228    5.012 -17.452  -3.159  1.00 31.68
BBBBATOM   4298  OE2 GLU B 228    5.154 -19.212  -4.471  1.00 32.04
BBBBATOM   4299  C   GLU B 228    6.746 -21.327  -0.994  1.00 27.95
BBBBATOM   4300  O   GLU B 228    7.511 -20.383  -0.787  1.00 27.32
BBBBATOM   4301  N   GLN B 229    6.374 -22.178  -0.041  1.00 28.66
BBBBATOM   4302  CA  GLN B 229    6.853 -22.046   1.329  1.00 28.38
BBBBATOM   4303  CB  GLN B 229    6.082 -22.990   2.261  1.00 31.03
BBBBATOM   4304  CG  GLN B 229    6.570 -22.946   3.700  1.00 35.48
BBBBATOM   4305  CD  GLN B 229    5.780 -23.860   4.615  1.00 38.01
BBBBATOM   4306  OE1 GLN B 229    4.548 -23.810   4.645  1.00 39.26
BBBBATOM   4307  NE2 GLN B 229    6.484 -24.697   5.370  1.00 38.61
BBBBATOM   4308  C   GLN B 229    8.338 -22.362   1.407  1.00 27.09
BBBBATOM   4309  O   GLN B 229    9.084 -21.697   2.124  1.00 28.29
BBBBATOM   4310  N   ALA B 230    8.771 -23.385   0.677  1.00 26.97
BBBBATOM   4311  CA  ALA B 230   10.185 -23.754   0.682  1.00 26.18
BBBBATOM   4312  CB  ALA B 230   10.412 -24.984  -0.184  1.00 25.07
BBBBATOM   4313  C   ALA B 230   11.054 -22.588   0.192  1.00 26.36
BBBBATOM   4314  O   ALA B 230   12.119 -22.317   0.755  1.00 25.04
BBBBATOM   4315  N   TYR B 231   10.605 -21.895  -0.854  1.00 25.85
BBBBATOM   4316  CA  TYR B 231   11.371 -20.766  -1.366  1.00 25.47
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BBBBATOM   4317  CB  TYR B 231     10.762 -20.248  -2.678  1.00 24.72
BBBBATOM   4318  CG  TYR B 231     11.236 -21.014  -3.905  1.00 23.66
BBBBATOM   4319  CD1 TYR B 231     12.546 -20.869  -4.381  1.00 23.97
BBBBATOM   4320  CE1 TYR B 231     13.006 -21.599  -5.488  1.00 21.40
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BBBBATOM   4322  CE2 TYR B 231     10.841 -22.641  -5.681  1.00 22.71
BBBBATOM   4323  CZ  TYR B 231     12.151 -22.480  -6.128  1.00 21.91
BBBBATOM   4324  OH  TYR B 231     12.600 -23.214  -7.199  1.00 21.69
BBBBATOM   4325  C   TYR B 231     11.450 -19.639  -0.336  1.00 26.53
BBBBATOM   4326  O   TYR B 231     12.498 -19.011  -0.175  1.00 26.32
BBBBATOM   4327  N   ALA B 232     10.345 -19.380   0.361  1.00 26.28
BBBBATOM   4328  CA  ALA B 232     10.342 -18.322   1.368  1.00 27.51
BBBBATOM   4329  CB  ALA B 232      8.930 -18.109   1.910  1.00 28.09
BBBBATOM   4330  C   ALA B 232     11.303 -18.695   2.499  1.00 28.03
BBBBATOM   4331  O   ALA B 232     12.069 -17.858   2.983  1.00 27.93
BBBBATOM   4332  N   GLU B 233     11.263 -19.958   2.911  1.00 29.43
BBBBATOM   4333  CA  GLU B 233     12.145 -20.441   3.966  1.00 30.87
BBBBATOM   4334  CB  GLU B 233     11.772 -21.877   4.344  1.00 33.60
BBBBATOM   4335  CG  GLU B 233     10.491 -21.973   5.170  1.00 37.67
BBBBATOM   4336  CD  GLU B 233     10.077 -23.404   5.461  1.00 40.35
BBBBATOM   4337  OE1 GLU B 233     10.964 -24.283   5.525  1.00 42.97
BBBBATOM   4338  OE2 GLU B 233      8.864 -23.649   5.641  1.00 41.95
BBBBATOM   4339  C   GLU B 233     13.606 -20.369   3.530  1.00 30.58
BBBBATOM   4340  O   GLU B 233     14.499 -20.202   4.359  1.00 30.82
BBBBATOM   4341  N   ALA B 234     13.850 -20.485   2.227  1.00 29.17
BBBBATOM   4342  CA  ALA B 234     15.215 -20.417   1.714  1.00 28.48
BBBBATOM   4343  CB  ALA B 234     15.310 -21.110   0.354  1.00 27.71
BBBBATOM   4344  C   ALA B 234     15.649 -18.961   1.588  1.00 27.73
BBBBATOM   4345  O   ALA B 234     16.787 -18.677   1.213  1.00 27.34
BBBBATOM   4346  N   GLY B 235     14.731 -18.045   1.890  1.00 26.74
BBBBATOM   4347  CA  GLY B 235     15.033 -16.627   1.815  1.00 26.23
BBBBATOM   4348  C   GLY B 235     14.946 -16.009   0.426  1.00 26.13
BBBBATOM   4349  O   GLY B 235     15.483 -14.924   0.198  1.00 25.67
BBBBATOM   4350  N   GLN B 236     14.284 -16.696  -0.502  1.00 25.36
BBBBATOM   4351  CA  GLN B 236     14.121 -16.198  -1.870  1.00 25.53
BBBBATOM   4352  CB  GLN B 236     14.940 -17.043  -2.852  1.00 25.84
BBBBATOM   4353  CG  GLN B 236     16.436 -17.074  -2.603  1.00 27.18
BBBBATOM   4354  CD  GLN B 236     17.080 -15.705  -2.661  1.00 28.96
BBBBATOM   4355  OE1 GLN B 236     16.686 -14.850  -3.456  1.00 30.03
BBBBATOM   4356  NE2 GLN B 236     18.092 -15.495  -1.829  1.00 29.39
BBBBATOM   4357  C   GLN B 236     12.641 -16.298  -2.232  1.00 24.12
BBBBATOM   4358  O   GLN B 236     12.262 -17.002  -3.167  1.00 23.31
BBBBATOM   4359  N   PRO B 237     11.783 -15.578  -1.497  1.00 24.40
BBBBATOM   4360  CD  PRO B 237     12.143 -14.580  -0.473  1.00 24.52
BBBBATOM   4361  CA  PRO B 237     10.336 -15.587  -1.720  1.00 24.65
BBBBATOM   4362  CB  PRO B 237      9.808 -14.798  -0.527  1.00 25.37
BBBBATOM   4363  CG  PRO B 237     10.862 -13.773  -0.340  1.00 25.24
BBBBATOM   4364  C   PRO B 237      9.837 -15.012  -3.043  1.00 25.33
BBBBATOM   4365  O   PRO B 237      8.720 -15.313  -3.465  1.00 24.93
BBBBATOM   4366  N   GLN B 238     10.663 -14.197  -3.690  1.00 24.47
BBBBATOM   4367  CA  GLN B 238     10.277 -13.558  -4.945  1.00 24.29
BBBBATOM   4368  CB  GLN B 238     11.281 -12.455  -5.306  1.00 23.76
BBBBATOM   4369  CG  GLN B 238     12.622 -12.945  -5.852  1.00 25.22
BBBBATOM   4370  CD  GLN B 238     13.535 -13.523  -4.783  1.00 26.90
BBBBATOM   4371  OE1 GLN B 238     13.188 -13.550  -3.600  1.00 28.05
BBBBATOM   4372  NE2 GLN B 238     14.712 -13.983  -5.195  1.00 25.61
BBBBATOM   4373  C   GLN B 238     10.108 -14.489  -6.143  1.00 23.41
BBBBATOM   4374  O   GLN B 238      9.485 -14.112  -7.139  1.00 20.49
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BBBBATOM   4377  CB  HIS B 239     11.432 -17.829  -7.008  1.00 22.41
BBBBATOM   4378  CG  HIS B 239     12.891 -17.488  -6.998  1.00 20.93
BBBBATOM   4379  CD2 HIS B 239     13.869 -17.774  -6.104  1.00 20.09
BBBBATOM   4380  ND1 HIS B 239     13.488 -16.743  -7.992  1.00 20.30
BBBBATOM   4381  CE1 HIS B 239     14.769 -16.582  -7.711  1.00 22.38
BBBBATOM   4382  NE2 HIS B 239     15.025 -17.197  -6.569  1.00 19.62
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BBBBATOM   4383  C   HIS B 239      9.076 -17.024  -7.433  1.00 22.98
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BBBBATOM   4391  NZ  LYS B 240      3.478 -16.129 -12.884  1.00 21.82
BBBBATOM   4392  C   LYS B 240      7.149 -19.091  -9.046  1.00 23.38
BBBBATOM   4393  O   LYS B 240      7.922 -19.871  -9.607  1.00 23.06
BBBBATOM   4394  N   VAL B 241      6.075 -19.497  -8.378  1.00 23.98
BBBBATOM   4395  CA  VAL B 241      5.740 -20.911  -8.277  1.00 23.78
BBBBATOM   4396  CB  VAL B 241      5.858 -21.428  -6.833  1.00 24.03
BBBBATOM   4397  CG1 VAL B 241      5.548 -22.923  -6.803  1.00 24.14
BBBBATOM   4398  CG2 VAL B 241      7.242 -21.144  -6.281  1.00 23.49
BBBBATOM   4399  C   VAL B 241      4.299 -21.136  -8.723  1.00 24.15
BBBBATOM   4400  O   VAL B 241      3.380 -20.528  -8.184  1.00 24.63
BBBBATOM   4401  N   THR B 242      4.103 -22.000  -9.710  1.00 24.22
BBBBATOM   4402  CA  THR B 242      2.758 -22.301 -10.177  1.00 25.93
BBBBATOM   4403  CB  THR B 242      2.513 -21.812 -11.615  1.00 25.89
BBBBATOM   4404  OG1 THR B 242      3.466 -22.419 -12.492  1.00 27.48
BBBBATOM   4405  CG2 THR B 242      2.639 -20.299 -11.697  1.00 26.82
BBBBATOM   4406  C   THR B 242      2.555 -23.809 -10.135  1.00 26.29
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BBBBATOM   4408  N   GLU B 243      1.319 -24.228  -9.898  1.00 26.70
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BBBBATOM   4411  CG  GLU B 243     -0.831 -27.218  -8.962  1.00 30.88
BBBBATOM   4412  CD  GLU B 243     -2.297 -27.341  -8.583  1.00 33.00
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BBBBATOM   4414  OE2 GLU B 243     -3.063 -26.383  -8.827  1.00 32.17
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BBBBATOM   4420  CG  PHE B 244     -1.110 -27.531 -13.307  1.00 30.15
BBBBATOM   4421  CD1 PHE B 244     -0.622 -28.817 -13.107  1.00 32.26
BBBBATOM   4422  CD2 PHE B 244     -2.318 -27.172 -12.716  1.00 31.10
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BBBBATOM   4425  CZ  PHE B 244     -2.549 -29.371 -11.744  1.00 32.59
BBBBATOM   4426  C   PHE B 244      1.420 -24.915 -14.507  1.00 25.60
BBBBATOM   4427  O   PHE B 244      1.604 -23.794 -14.053  1.00 24.93
BBBBATOM   4428  N   ILE B 245      1.591 -25.223 -15.786  1.00 27.02
BBBBATOM   4429  CA  ILE B 245      1.932 -24.242 -16.802  1.00 28.48
BBBBATOM   4430  CB  ILE B 245      3.441 -24.226 -17.159  1.00 28.41
BBBBATOM   4431  CG2 ILE B 245      3.676 -23.348 -18.399  1.00 27.05
BBBBATOM   4432  CG1 ILE B 245      4.245 -23.663 -15.983  1.00 27.10
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BBBBATOM   4434  C   ILE B 245      1.127 -24.721 -18.000  1.00 30.75
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BBBBATOM   4436  N   ASP B 246      0.071 -23.997 -18.331  1.00 33.46
BBBBATOM   4437  CA  ASP B 246     -0.754 -24.396 -19.457  1.00 36.00
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BBBBATOM   4444  N   ASP B 247      0.582 -22.876 -20.794  1.00 33.18
BBBBATOM   4445  CA  ASP B 247      1.245 -22.392 -21.999  1.00 30.74
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BBBBATOM   4451  O   ASP B 247       3.494 -21.695 -21.525  1.00 27.28
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BBBBATOM   4455  CG  MET B 248       4.952 -26.469 -21.150  1.00 34.21
BBBBATOM   4456  SD  MET B 248       6.277 -25.936 -20.049  1.00 38.21
BBBBATOM   4457  CE  MET B 248       5.611 -26.499 -18.479  1.00 37.90
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BBBBATOM   4460  N   ALA B 249       4.827 -23.009 -24.279  1.00 26.23
BBBBATOM   4461  CA  ALA B 249       5.512 -22.216 -25.290  1.00 24.67
BBBBATOM   4462  CB  ALA B 249       4.625 -22.069 -26.537  1.00 25.39
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BBBBATOM   4466  CA  ALA B 250       5.188 -18.933 -23.390  1.00 21.78
BBBBATOM   4467  CB  ALA B 250       3.898 -18.376 -22.797  1.00 23.21
BBBBATOM   4468  C   ALA B 250       6.277 -19.011 -22.313  1.00 21.84
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BBBBATOM   4478  CG  TYR B 252       9.662 -24.100 -23.505  1.00 23.34
BBBBATOM   4479  CD1 TYR B 252       9.003 -25.065 -24.261  1.00 22.88
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BBBBATOM   4481  CD2 TYR B 252      10.288 -24.505 -22.319  1.00 22.30
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BBBBATOM   4483  CZ  TYR B 252       9.590 -26.772 -22.687  1.00 24.26
BBBBATOM   4484  OH  TYR B 252       9.554 -28.088 -22.305  1.00 25.57
BBBBATOM   4485  C   TYR B 252      10.566 -20.354 -23.516  1.00 23.57
BBBBATOM   4486  O   TYR B 252      11.784 -20.180 -23.550  1.00 23.91
BBBBATOM   4487  N   ALA B 253       9.699 -19.473 -24.007  1.00 23.22
BBBBATOM   4488  CA  ALA B 253      10.131 -18.224 -24.636  1.00 23.54
BBBBATOM   4489  CB  ALA B 253       8.931 -17.512 -25.275  1.00 24.59
BBBBATOM   4490  C   ALA B 253      10.783 -17.305 -23.617  1.00 23.30
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BBBBATOM   4492  N   TRP B 254      10.299 -17.369 -22.379  1.00 20.49
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BBBBATOM   4494  CB  TRP B 254       9.808 -16.467 -20.151  1.00 19.57
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BBBBATOM   4496  CD2 TRP B 254      10.870 -16.796 -17.762  1.00 19.25
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BBBBATOM   4498  CE3 TRP B 254      10.939 -18.178 -17.543  1.00 19.18
BBBBATOM   4499  CD1 TRP B 254      10.591 -14.691 -18.470  1.00 19.03
BBBBATOM   4500  NE1 TRP B 254      11.185 -14.643 -17.226  1.00 20.30
BBBBATOM   4501  CZ2 TRP B 254      11.931 -16.382 -15.572  1.00 20.01
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BBBBATOM   4504  C   TRP B 254      12.156 -17.059 -20.755  1.00 19.33
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BBBBATOM   4518  O   ASP B 256      18.459 -20.929 -21.198  1.00 16.11
BBBBATOM   4519  N   VAL B 257      17.147 -21.216 -19.396  1.00 17.49
BBBBATOM   4520  CA  VAL B 257      17.535 -22.603 -19.194  1.00 18.53
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BBBBATOM   4523  CG2 VAL B 257      19.286 -24.129 -18.200  1.00 20.40
BBBBATOM   4524  C   VAL B 257      16.400 -23.363 -18.501  1.00 18.31
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BBBBATOM   4528  CB  VAL B 258      14.328 -26.100 -19.337  1.00 19.89
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BBBBATOM   4535  CB  VAL B 259      15.850 -27.483 -13.936  1.00 20.08
BBBBATOM   4536  CG1 VAL B 259      16.222 -28.689 -13.059  1.00 20.22
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BBBBATOM   4595  CA  SER B 268      12.411 -33.191 -28.567  1.00 21.96
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BBBBATOM   4732  OD1 ASP B 286      15.971 -50.338 -20.925  1.00 49.52
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BBBBATOM   4745  C   ARG B 287      17.449 -45.005 -19.180  1.00 33.59
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BBBBATOM   4981  CG2  THR B 318      24.784 -27.539 -14.655  1.00 27.49
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BBBBATOM   4983  O    THR B 318      26.085 -24.548 -14.465  1.00 26.71
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BBBBATOM   4985  CA   LEU B 319      23.883 -23.370 -13.357  1.00 25.21
BBBBATOM   4986  CB   LEU B 319      22.579 -23.090 -12.600  1.00 23.70
BBBBATOM   4987  CG   LEU B 319      21.496 -24.153 -12.803  1.00 23.20
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BBBBATOM   4989  CD2  LEU B 319      20.963 -24.065 -14.237  1.00 22.39
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BBBBATOM   4995  C    ALA B 320      27.549 -20.865 -13.010  1.00 24.21
BBBBATOM   4996  O    ALA B 320      28.091 -19.800 -13.281  1.00 24.35
BBBBATOM   4997  N    GLY B 321      27.878 -22.005 -13.601  1.00 24.35
BBBBATOM   4998  CA.  GLY B 321      28.934 -22.031 -14.591  1.00 24.34
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BBBBATOM   5003  CB   TRP B 322      25.499 -21.841 -17.858  1.00 20.09
BBBBATOM   5004  CG   TRP B 322      25.763 -23.318 -17.973  1.00 19.85
BBBBATOM   5005  CD2  TRP B 322      24.789 -24.370 -17.939  1.00 19.16
BBBBATOM   5006  CE2  TRP B 322      25.479 -25.584 -18.164  1.00 20.31
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BBBBATOM   5025  CD   ARG B 324      22.508 -12.662 -20.220  1.00 22.13
BBBBATOM   5026  NE   ARG B 324      21.345 -12.641 -19.331  1.00 21.36
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BBBBATOM   5028  NH1  ARG B 324      20.206 -14.224 -20.549  1.00 20.63
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BBBBATOM   5030  C    ARG B 324      25.288 -16.145 -22.481  1.00 17.79
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BBBBATOM   5040  O    GLU B 325      26.838 -18.428 -25.172  1.00 15.39
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BBBBATOM   5050  CB  LEU B 327      22.791 -19.514 -21.791  1.00 17.35
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BBBBATOM   5052  CD1 LEU B 327      22.192 -18.930 -19.416  1.00 14.82
BBBBATOM   5053  CD2 LEU B 327      22.361 -21.312 -20.129  1.00 18.13
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BBBBATOM   5055  O   LEU B 327      22.352 -20.899 -24.692  1.00 16.08
BBBBATOM   5056  N   LEU B 328      23.584 -19.014 -24.845  1.00 17.87
BBBBATOM   5057  CA  LEU B 328      23.175 -18.745 -26.222  1.00 17.39
BBBBATOM   5058  CB  LEU B 328      23.706 -17.379 -26.690  1.00 17.84
BBBBATOM   5059  CG  LEU B 328      23.475 -17.021 -28.173  1.00 18.65
BBBBATOM   5060  CD1 LEU B 328      21.988 -17.112 -28.494  1.00 16.92
BBBBATOM   5061  CD2 LEU B 328      23.984 -15.608 -28.460  1.00 18.47
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BBBBATOM   5064  N   THR B 329      24.977 -20.244 -26.910  1.00 20.12
BBBBATOM   5065  CA  THR B 329      25.567 -21.335 -27.688  1.00 21.30
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BBBBATOM   5075  SD  MET B 330      24.805 -24.609 -21.855  1.00 22.76
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BBBBATOM   5095  CB  ARG B 333      24.117 -26.789 -29.427  1.00 25.03
BBBBATOM   5096  CG  ARG B 333      25.503 -26.222 -29.737  1.00 26.79
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BBBBATOM   5115  CZ  ARG B 335      13.607 -22.469 -33.301  1.00 35.57
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BBBBATOM   5155  OD1 ASP B 341      11.125 -31.907 -40.443  1.00 37.17
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BBBBATOM   5164  N   THR B 343       6.441 -35.177 -37.427  1.00 28.28
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BBBBATOM   5168  CG2 THR B 343       2.628 -35.330 -37.528  1.00 28.54
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BBBBATOM   5187  NH1 ARG B 345      14.514 -35.782 -41.031  1.00 46.05
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BBBBATOM   5191  N   VAL B 346       7.086 -38.818 -40.670  1.00 29.72
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BBBBATOM   5194  CG1 VAL B 346       5.612 -41.680 -38.625  1.00 27.30
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BBBBATOM   5196  C   VAL B 346       5.361 -40.435 -41.252  1.00 28.33
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BBBBATOM   5211  N   GLU B 349       6.366 -41.212 -44.794  1.00 35.20
BBBBATOM   5212  CA  GLU B 349       6.954 -42.540 -44.956  1.00 34.86
BBBBATOM   5213  CB  GLU B 349       8.004 -42.814 -43.879  1.00 34.59
BBBBATOM   5214  CG  GLU B 349       9.404 -42.385 -44.259  1.00 38.16
BBBBATOM   5215  CD  GLU B 349       9.865 -42.992 -45.579  1.00 38.74
BBBBATOM   5216  OE1 GLU B 349       9.806 -44.232 -45.735  1.00 40.12
BBBBATOM   5217  OE2 GLU B 349      10.292 -42.225 -46.461  1.00 39.64
BBBBATOM   5218  C   GLU B 349       5.872 -43.607 -44.895  1.00 33.96
BBBBATOM   5219  O   GLU B 349       5.942 -44.621 -45.591  1.00 33.99
BBBBATOM   5220  N   VAL B 350       4.875 -43.377 -44.051  1.00 33.91
BBBBATOM   5221  CA  VAL B 350       3.767 -44.306 -43.919  1.00 33.79
BBBBATOM   5222  CB  VAL B 350       2.848 -43.907 -42.744  1.00 33.70
BBBBATOM   5223  CG1 VAL B 350       1.554 -44.695 -42.798  1.00 32.22
BBBBATOM   5224  CG2 VAL B 350       3.568 -44.154 -41.425  1.00 32.24
BBBBATOM   5225  C   VAL B 350       2.969 -44.274 -45.217  1.00 34.78
BBBBATOM   5226  O   VAL B 350       2.411 -45.285 -45.645  1.00 34.85
BBBBATOM   5227  N   SER B 351       2.925 -43.102 -45.844  1.00 35.34
BBBBATOM   5228  CA  SER B 351       2.196 -42.946 -47.095  1.00 36.67
BBBBATOM   5229  CB  SER B 351       2.024 -41.462 -47.425  1.00 37.32
BBBBATOM   5230  OG  SER B 351       1.241 -41.292 -48.590  1.00 37.74
BBBBATOM   5231  C   SER B 351       2.958 -43.639 -48.222  1.00 37.35
BBBBATOM   5232  O   SER B 351       2.365 -44.309 -49.064  1.00 36.85
BBBBATOM   5233  N   ARG B 352       4.277 -43.482 -48.223  1.00 37.89
BBBBATOM   5234  CA  ARG B 352       5.114 -44.088 -49.251  1.00 40.03
BBBBATOM   5235  CB  ARG B 352       6.557 -43.600 -49.114  1.00 41.58
BBBBATOM   5236  CG  ARG B 352       7.470 -44.069 -50.232  1.00 44.46
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BBBBATOM   5238  NE  ARG B 352       9.097 -45.271 -48.832  1.00 49.57
BBBBATOM   5239  CZ  ARG B 352      10.234 -45.524 -48.191  1.00 50.54
BBBBATOM   5240  NH1 ARG B 352      11.287 -44.738 -48.372  1.00 50.88
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BBBBATOM   5243  O   ARG B 352       5.101 -46.292 -50.204  1.00 39.84
BBBBATOM   5244  N   VAL B 353       5.096 -46.143 -47.955  1.00 41.33
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BBBBATOM   5246  CB  VAL B 353       5.446 -47.927 -46.271  1.00 42.54
BBBBATOM   5247  CG1 VAL B 353       5.279 -49.420 -46.014  1.00 42.05
BBBBATOM   5248  CG2 VAL B 353       6.879 -47.509 -45.987  1.00 41.86
BBBBATOM   5249  C   VAL B 353       3.742 -48.206 -48.095  1.00 43.85
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BBBBATOM   5252  CA  ALA B 354       1.336 -47.957 -48.212  1.00 47.24
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BBBBATOM   5255  O   ALA B 354       0.531 -48.780 -50.324  1.00 48.48
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BBBBATOM   5257  CA  ARG B 355       2.035 -46.964 -51.824  1.00 52.71
BBBBATOM   5258  CB  ARG B 355       2.658 -45.633 -52.264  1.00 53.58
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BBBBATOM   5263  NH1 ARG B 355      -1.758 -42.896 -53.252  1.00 58.53
BBBBATOM   5264  NH2 ARG B 355      -1.519 -41.186 -51.738  1.00 58.87
BBBBATOM   5265  C   ARG B 355       2.899 -48.099 -52.366  1.00 53.41
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BBBBATOM   5268  CA  ALA B 356       4.453 -49.913 -51.809  1.00 54.93
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BBBBATOM   5270  C   ALA B 356       5.611 -49.417 -52.671  1.00 55.63
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BBBBATOM   5273  CA  LEU B 357       7.023 -47.522 -53.289  1.00 57.81
BBBBATOM   5274  CB  LEU B 357       6.871 -45.997 -53.290  1.00 58.04
BBBBATOM   5275  CG  LEU B 357       5.595 -45.422 -53.915  1.00 58.29
BBBBATOM   5276  CD1 LEU B 357       5.624 -43.903 -53.820  1.00 58.36
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WATR
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WATR
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WATR
ATOM   5285  OH2 WAT W   7       2.329 -28.724 -15.978  1.00 27.32
WATR
ATOM   5286  OH2 WAT W   8       9.484 -48.435 -27.938  1.00 23.67
WATR
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WATR
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WATR
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WATR
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WATR
ATOM   5292  OH2 WAT W  14       4.845 -57.924 -27.444  1.00 24.35
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WATR
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WATRATOM   5356  OH2 WAT W  78      11.725 -25.065 -33.817  1.00 43.79
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WATRATOM   5359  OH2 WAT W  81      -2.250  -0.253  -1.741  1.00 29.99
WATRATOM   5360  OH2 WAT W  82      -7.300  12.943   8.415  1.00 32.39
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WATRATOM   5363  OH2 WAT W  85      10.070 -57.496 -44.450  1.00 48.39
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WATRATOM   5365  OH2 WAT W  87      -1.967 -32.372 -38.643  1.00 31.55
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WATRATOM   5397  OH2 WAT W 119     -5.862   6.629   4.446  1.00 39.57
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WATRATOM   5401  OH2 WAT W 123     15.481   1.078  -4.048  1.00 32.28
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WATRATOM   5405  OH2 WAT W 127      9.994 -12.069 -21.013  1.00 32.21
WATRATOM   5406  OH2 WAT W 128     17.433 -42.825 -16.713  1.00 31.02
WATRATOM   5407  OH2 WAT W 129    -15.855  20.882  21.019  1.00 44.11
WATRATOM   5408  OH2 WAT W 130     -6.351  -7.687 -14.067  1.00 35.04
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WATRATOM   5410  OH2 WAT W 132     13.526 -34.593 -31.844  1.00 31.12
WATRATOM   5411  OH2 WAT W 133      9.992 -41.228 -23.098  1.00 26.45
WATRATOM   5412  OH2 WAT W 134      8.434  18.132  16.019  1.00 32.97
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WATRATOM   5414  OH2 WAT W 136    -14.502   9.100  12.433  1.00 43.21
WATRATOM   5415  OH2 WAT W 137     14.394 -43.675 -17.325  1.00 32.32
WATRATOM   5416  OH2 WAT W 138     -4.809 -30.333 -46.416  1.00 42.65
WATRATOM   5417  OH2 WAT W 139     18.861 -35.072 -35.671  1.00 43.56
WATRATOM   5418  OH2 WAT W 140    -10.162 -60.139 -32.862  1.00 35.41
WATRATOM   5419  OH2 WAT W 141      6.740 -32.411 -35.303  1.00 38.57
WATRATOM   5420  OH2 WAT W 142    -12.257 -60.854 -39.307  1.00 32.90
WATRATOM   5421  OH2 WAT W 143     18.910 -40.984 -13.084  1.00 43.43
WATRATOM   5422  OH2 WAT W 144     18.857 -49.375 -28.645  1.00 31.34
WATRATOM   5423  OH2 WAT W 145      0.235 -17.424 -16.608  1.00 38.85
WATRATOM   5424  OH2 WAT W 146     14.236 -11.252 -24.086  1.00 27.79
WATRATOM   5425  OH2 WAT W 147     31.513 -22.336 -22.128  1.00 43.18
WATRATOM   5426  OH2 WAT W 148     -5.314 -70.396 -26.090  1.00 43.91
WATRATOM   5427  OH2 WAT W 149     -7.717 -64.969 -36.808  1.00 26.30
WATRATOM   5428  OH2 WAT W 150     22.584 -12.594  -4.179  1.00 46.91
WATRATOM   5429  OH2 WAT W 151    -12.388   9.493  36.619  1.00 32.82
WATRATOM   5430  OH2 WAT W 152    -14.517  16.479  37.760  1.00 39.52
WATRATOM   5431  OH2 WAT W 153    -10.095 -34.647 -29.068  1.00 41.08
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WATRATOM   5432  OH2 WAT W 154     -5.233  -4.134  31.160  1.00 35.31
WATRATOM   5433  OH2 WAT W 155     -6.322  11.278  -1.883  1.00 35.75
WATRATOM   5434  OH2 WAT W 156     10.262  -9.572 -16.736  1.00 42.40
WATRATOM   5435  OH2 WAT W 157     22.929 -10.414 -23.566  1.00 36.66
WATRATOM   5436  OH2 WAT W 158    -15.987   3.994  16.559  1.00 37.22
WATRATOM   5437  OH2 WAT W 159     13.385 -44.923 -46.826  1.00 41.55
WATRATOM   5438  OH2 WAT W 160     26.508 -13.616 -18.049  1.00 25.93
WATRATOM   5439  OH2 WAT W 161      4.671 -66.907 -17.861  1.00 31.54
WATRATOM   5440  OH2 WAT W 162    -12.589  12.262  11.825  1.00 32.71
WATRATOM   5441  OH2 WAT W 163     13.899 -62.269 -25.144  1.00 30.71
WATRATOM   5442  OH2 WAT W 164    -31.053  15.663  19.272  1.00 30.19
WATRATOM   5443  OH2 WAT W 165      9.797 -47.899 -25.140  1.00 26.79
WATRATOM   5444  OH2 WAT W 166      0.877 -51.774 -25.619  1.00 30.02
WATRATOM   5445  OH2 WAT W 167    -17.088  16.246  37.180  1.00 25.63
WATRATOM   5446  OH2 WAT W 168      0.855 -52.086 -22.078  1.00 40.99
WATRATOM   5447  OH2 WAT W 169    -14.873  18.295  21.203  1.00 40.28
WATRATOM   5448  OH2 WAT W 170     11.913 -62.134 -35.641  1.00 41.33
WATRATOM   5449  OH2 WAT W 171     25.783 -23.984 -33.162  1.00 44.03
WATRATOM   5450  OH2 WAT W 172      7.169 -50.047 -23.737  1.00 47.85
WATRATOM   5451  OH2 WAT W 173     20.074 -42.845 -14.939  1.00 32.87
WATRATOM   5452  OH2 WAT W 174      8.765   5.909   9.193  1.00 34.30
WATRATOM   5453  OH2 WAT W 175     -4.953 -64.494 -45.351  1.00 47.11
WATRATOM   5454  OH2 WAT W 176     11.889 -61.263 -22.531  1.00 36.63
WATRATOM   5455  OH2 WAT W 177      2.149 -49.169 -24.836  1.00 39.21
WATRATOM   5456  OH2 WAT W 178    -14.051   6.399  13.353  1.00 39.89
WATRATOM   5457  OH2 WAT W 179      8.488 -46.760 -23.118  1.00 45.24
WATRATOM   5458  OH2 WAT W 180     -1.152 -23.348 -11.975  1.00 30.36
WATRATOM   5459  OH2 WAT W 181     -7.002   3.531   7.051  1.00 44.50
WATRATOM   5460  OH2 WAT W 182    -12.320 -54.772 -29.990  1.00 38.61
WATRATOM   5461  OH2 WAT W 183      6.790 -54.559 -47.733  1.00 44.05
WATRATOM   5462  OH2 WAT W 184     26.305 -38.240 -19.177  1.00 39.53
WATRATOM   5463  OH2 WAT W 185     20.402 -58.179 -34.391  1.00 46.11
WATRATOM   5464  OH2 WAT W 186      8.061 -31.341 -19.653  1.00 41.37
WATRATOM   5465  OH2 WAT W 187     -7.549 -15.619  -5.482  1.00 40.60
WATRATOM   5466  OH2 WAT W 188    -31.099  11.941  25.471  1.00 38.80
WATRATOM   5467  OH2 WAT W 189     28.566 -25.441 -15.103  1.00 34.75
WATRATOM   5468  OH2 WAT W 190     -5.613 -40.109 -50.158  1.00 49.21
WATRATOM   5469  OH2 WAT W 191     17.024 -13.428   1.709  1.00 39.93
WATRATOM   5470  OH2 WAT W 192    -22.114  10.176  37.673  1.00 32.53
WATRATOM   5471  OH2 WAT W 193     10.204 -29.330 -20.066  1.00 27.24
WATRATOM   5472  OH2 WAT W 194     27.893 -25.793 -21.862  1.00 38.97
WATRATOM   5473  OH2 WAT W 195     -5.582  17.681  32.898  1.00 43.64
WATRATOM   5474  OH2 WAT W 196     23.004 -45.224 -27.870  1.00 43.04
WATRATOM   5475  OH2 WAT W 197      5.189 -58.857 -25.016  1.00 28.15
WATRATOM   5476  OH2 WAT W 198     -7.740 -56.165 -24.052  1.00 35.98
WATRATOM   5477  OH2 WAT W 199     -8.156  24.723  26.733  1.00 45.54
WATRATOM   5478  OH2 WAT W 200     23.286 -32.333 -33.400  1.00 38.12
WATRATOM   5479  OH2 WAT W 201     30.646 -14.180 -20.528  1.00 31.01
WATRATOM   5480  OH2 WAT W 202     -8.238  -4.609  29.299  1.00 39.76
WATRATOM   5481  OH2 WAT W 203     19.370   0.814  -7.532  1.00 35.83
WATRATOM   5482  OH2 WAT W 204      0.885 -27.619  -1.442  1.00 47.04
WATRATOM   5483  OH2 WAT W 205     16.084 -56.649 -26.382  1.00 45.97
WATRATOM   5484  OH2 WAT W 206     -0.698 -19.360  -9.869  1.00 37.53
WATRATOM   5485  OH2 WAT W 207      0.682 -14.985 -15.794  1.00 33.35
WATRATOM   5486  OH2 WAT W 208      1.646  17.427  31.991  1.00 40.39
WATRATOM   5487  OH2 WAT W 209    -21.611   1.533  20.359  1.00 31.04
WATRATOM   5488  OH2 WAT W 210     -5.143 -55.137 -45.825  1.00 30.17
WATRATOM   5489  OH2 WAT W 211     -9.645  13.045  37.660  1.00 42.93
WATRATOM   5490  OH2 WAT W 212     22.096 -11.242 -30.224  1.00 48.12
WATRATOM   5491  OH2 WAT W 213     -5.759   2.610 -15.984  1.00 41.67
WATRATOM   5492  OH2 WAT W 214     -4.323   7.731  -7.331  1.00 37.92
WATRATOM   5493  OH2 WAT W 215     -5.450   7.197  10.632  1.00 33.99
WATRATOM   5494  OH2 WAT W 216      2.330 -32.635 -34.500  1.00 38.85
WATRATOM   5495  OH2 WAT W 217    -26.827  16.219  13.451  1.00 38.12
WATRATOM   5496  OH2 WAT W 218     10.887 -51.427 -23.191  1.00 39.81
WATRATOM   5497  OH2 WAT W 219     -9.020  19.746  -3.698  1.00 46.58
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WATRATOM   5498  OH2 WAT W 220      9.054    6.622   -0.709  1.00 34.14
WATRATOM   5499  OH2 WAT W 221      4.173   -7.985  -23.786  1.00 32.75
WATRATOM   5500  OH2 WAT W 222      0.983   16.806    3.910  1.00 40.83
WATRATOM   5501  OH2 WAT W 223      2.222  -16.848   -6.783  1.00 33.50
WATRATOM   5502  OH2 WAT W 224     13.627    1.072  -15.114  1.00 37.51
WATRATOM   5503  OH2 WAT W 225     12.533  -14.212   -9.007  1.00 38.40
WATRATOM   5504  OH2 WAT W 226      1.404   -7.852    5.396  1.00 38.55
WATRATOM   5505  OH2 WAT W 227     31.159  -24.354  -31.143  1.00 37.67
WATRATOM   5506  OH2 WAT W 228    -13.047  -60.728  -42.282  1.00 42.18
WATRATOM   5507  OH2 WAT W 229      8.956  -37.681  -16.765  1.00 41.45
WATRATOM   5508  OH2 WAT W 230     28.749  -13.637  -16.860  1.00 42.34
WATRATOM   5509  OH2 WAT W 231     -4.461   19.451    8.684  1.00 36.17
WATRATOM   5510  OH2 WAT W 232     -9.785  -66.504  -35.701  1.00 44.07
WATRATOM   5511  OH2 WAT W 233     10.673  -41.619  -20.678  1.00 36.58
WATRATOM   5512  OH2 WAT W 234    -15.694    1.684   32.613  1.00 44.04
WATRATOM   5513  OH2 WAT W 235      3.345    1.229    9.738  1.00 35.70
WATRATOM   5514  OH2 WAT W 236     -6.256  -68.913  -30.401  1.00 36.72
WATRATOM   5515  OH2 WAT W 237     28.344  -21.326  -30.399  1.00 36.45
WATRATOM   5516  OH2 WAT W 238      2.876  -34.368  -17.344  1.00 42.48
WATRATOM   5517  OH2 WAT W 239     15.355  -11.202    2.371  1.00 38.84
WATRATOM   5518  OH2 WAT W 240     27.066  -22.336   -6.437  1.00 37.37
WATRATOM   5519  OH2 WAT W 241      2.222   18.464   26.994  1.00 35.75
WATRATOM   5520  OH2 WAT W 242     15.052   -9.829  -31.019  1.00 44.31
WATRATOM   5521  OH2 WAT W 243     10.351  -67.649  -21.184  1.00 35.79
WATRATOM   5522  OH2 WAT W 244    -13.173   14.269   38.605  1.00 41.50
WATRATOM   5523  OH2 WAT W 245     -7.569    9.658    0.793  1.00 37.62
WATRATOM   5524  OH2 WAT W 246     -2.167  -47.395  -19.605  1.00 45.90
WATRATOM   5525  OH2 WAT W 247      7.166    2.400   15.830  1.00 42.90
WATRATOM   5526  OH2 WAT W 248    -11.231  -10.901  -10.057  1.00 45.28
WATRATOM   5527  OH2 WAT W 249      5.684  -16.094  -26.796  1.00 44.76
WATRATOM   5528  OH2 WAT W 250     -4.745    3.667  -18.932  1.00 46.20
WATRATOM   5529  OH2 WAT W 251     -0.505  -22.136   -9.079  1.00 42.89
WATRATOM   5530  OH2 WAT W 252     16.668  -37.987   -7.767  1.00 35.76
WATRATOM   5531  OH2 WAT W 253      2.454  -18.256  -26.130  1.00 43.33
WATRATOM   5532  OH2 WAT W 254     -8.367  -39.960  -21.638  1.00 43.07
WATRATOM   5533  OH2 WAT W 255     15.642    7.805    9.633  1.00 47.78
WATRATOM   5534  OH2 WAT W 256     13.660  -24.331    1.932  1.00 42.50
WATRATOM   5535  OH2 WAT W 257     11.567   -6.104  -23.359  1.00 37.10
WATRATOM   5536  OH2 WAT W 258     18.941  -16.698    0.528  1.00 40.97
WATRATOM   5537  OH2 WAT W 259    -11.441  -63.514  -39.126  1.00 43.17
WATRATOM   5538  OH2 WAT W 260     28.664  -39.605  -22.853  1.00 42.65
WATRATOM   5539  OH2 WAT W 261      6.795   -6.961   31.114  1.00 38.28
WATRATOM   5540  OH2 WAT W 262      7.077  -14.349  -24.858  1.00 41.00
WATRATOM   5541  OH2 WAT W 263     -2.259  -48.991  -29.099  1.00 34.96
WATRATOM   5542  OH2 WAT W 264     21.812  -44.128  -35.641  1.00 44.51
WATRATOM   5543  OH2 WAT W 265    -27.570    4.389   13.296  1.00 48.63
WATRATOM   5544  OH2 WAT W 266     13.573  -27.185    0.220  1.00 43.56
WATRATOM   5545  OH2 WAT W 267     16.549    8.451  -13.582  1.00 44.84
WATRATOM   5546  OH2 WAT W 268     -9.142    9.107   36.872  1.00 37.66
WATRATOM   5547  OH2 WAT W 269      5.648  -11.797  -24.893  1.00 45.79
WATRATOM   5548  OH2 WAT W 270      3.619  -14.850  -23.652  1.00 34.09
WATRATOM   5549  OH2 WAT W 271     -8.129  -11.098  -16.064  1.00 39.37
WATRATOM   5550  OH2 WAT W 272    -17.342    8.563    9.979  1.00 46.38
WATRATOM   5551  OH2 WAT W 273      8.798  -36.348  -46.119  1.00 37.71
WATRATOM   5552  OH2 WAT W 274      9.190  -10.509  -35.865  1.00 45.80
WATRATOM   5553  OH2 WAT W 275     13.545  -13.441    3.898  1.00 42.83
WATRATOM   5554  OH2 WAT W 276     -7.844    0.944   -2.560  1.00 46.27
WATRATOM   5555  OH2 WAT W 277      0.478  -47.721  -55.170  1.00 46.25
WATRATOM   5556  OH2 WAT W 278     24.658  -18.359  -11.005  1.00 36.33
WATRATOM   5557  OH2 WAT W 279     -4.675   21.561   12.155  1.00 37.17
WATRATOM   5558  OH2 WAT W 280      0.382   20.486    4.930  1.00 41.40
WATRATOM   5559  OH2 WAT W 281      5.919   18.010   25.033  1.00 41.72
WATRATOM   5560  OH2 WAT W 282     -2.987  -63.751  -22.983  1.00 43.76
WATRATOM   5561  OH2 WAT W 283      8.990  -33.134  -17.898  1.00 40.17
WATRATOM   5562  OH2 WAT W 284      0.155  -61.872  -48.384  1.00 49.87
WATRATOM   5563  OH2 WAT W 285    -10.443  -56.965  -24.681  1.00 48.02
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WATRATOM    5564  OH2 WAT W 286      18.915 -33.048  -3.930  1.00 37.81
WATRATOM    5565  OH2 WAT W 287     -16.181  11.706  12.277  1.00 41.77
WATRATOM    5566  OH2 WAT W 288       7.197   7.180  10.953  1.00 46.19
WATRATOM    5567  OH2 WAT W 289      31.934 -26.155 -26.053  1.00 38.77
WATRATOM    5568  OH2 WAT W 290     -15.232  -0.248  11.315  1.00 40.14
WATRATOM    5569  OH2 WAT W 291       9.450 -27.963  -1.396  1.00 41.29
WATRATOM    5570  OH2 WAT W 292      -1.800  13.139  -9.983  1.00 41.60
WATRATOM    5571  OH2 WAT W 293      -7.766   5.988   9.798  1.00 40.11
WATRATOM    5572  OH2 WAT W 294       7.973   4.338  14.321  1.00 39.97
WATRATOM    5573  OH2 WAT W 295      23.449 -40.563 -27.347  1.00 40.59
WATRATOM    5574  OH2 WAT W 296      -3.537 -28.260 -15.925  1.00 42.10
WATRATOM    5575  OH2 WAT W 297      28.052 -32.620 -12.168  1.00 48.03
WATRATOM    5576  OH2 WAT W 298      20.655 -43.315 -28.829  1.00 40.17
WATR
ATOM    5577  S   SO4 S   1       1.273 -70.953 -23.009  1.00 22.99
SO4
ATOM    5578  O1  SO4 S   1       1.720 -71.882 -24.053  1.00 21.18
SO4
ATOM    5579  O2  SO4 S   1       0.908 -69.659 -23.626  1.00 22.47
SO4
ATOM    5580  O3  SO4 S   1       2.337 -70.752 -22.018  1.00 23.88
SO4
ATOM    5581  O4  SO4 S   1       0.088 -71.522 -22.328  1.00 22.50
SO4
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TABLE 2 ATOMIC COORDINATES OF E.COLI MURG C-ALPHA BACKBONE ATOMS

ATOM	2649	CA	LYS	B	7	-6.512	-45.403	-47.519	1.00	45.28	BBBB
ATOM	2651	CA	ARG	B	8	-6.682	-47.303	-44.240	1.00	38.63	BBBB
ATOM	2662	CA	LEU	B	9	-4.094	-47.039	-41.477	1.00	30.88	BBBB
ATOM	2670	CA	MET	B	10	-4.048	-49.055	-38.275	1.00	26.66	BBBB
ATOM	2678	CA	VAL	B	11	-1.982	-47.605	-35.449	1.00	23.16	BBBB
ATOM	2685	CA	MET	B	12	-0.523	-49.707	-32.613	1.00	24.54	BBBB
ATOM	2693	CA	ALA	B	13	0.508	-47.410	-29.752	1.00	29.43	BBBB
ATOM	2698	CA	GLY	B	14	-0.513	-47.804	-26.120	1.00	33.82	BBBB
ATOM	2702	CA	GLY	B	15	-0.700	-45.047	-23.536	1.00	36.08	BBBB
ATOM	2706	CA	THR	B	16	1.920	-46.787	-21.421	1.00	38.51	BBBB
ATOM	2713	CA	GLY	B	17	5.367	-45.567	-22.392	1.00	36.57	BBBB
ATOM	2717	CA	GLY	B	18	3.631	-42.529	-23.872	1.00	33.48	BBBB
ATOM	2721	CA	HIS	B	19	3.548	-43.865	-27.435	1.00	28.22	BBBB
ATOM	2731	CA	VAL	B	20	-0.098	-42.894	-27.965	1.00	27.77	BBBB
ATOM	2738	CA	PHE	B	21	0.517	-39.136	-28.160	1.00	29.00	BBBB
ATOM	2750	CA	PRO	B	22	2.986	-39.252	-31.086	1.00	26.12	BBBB
ATOM	2756	CA	GLY	B	23	0.787	-41.864	-32.752	1.00	25.07	BBBB
ATOM	2760	CA	LEU	B	24	-2.201	-39.551	-32.401	1.00	25.32	BBBB
ATOM	2768	CA	ALA	B	25	-0.197	-36.754	-34.013	1.00	25.94	BBBB
ATOM	2773	CA	VAL	B	26	0.466	-38.955	-37.056	1.00	25.70	BBBB
ATOM	2780	CA	ALA	B	27	-3.116	-40.222	-37.199	1.00	26.15	BBBB
ATOM	2785	CA	HIS	B	28	-4.574	-36.702	-37.190	1.00	29.32	BBBB
ATOM	2795	CA	HIS	B	29	-2.070	-35.623	-39.806	1.00	32.38	BBBB
ATOM	2805	CA	LEU	B	30	-3.136	-38.417	-42.162	1.00	32.00	BBBB
ATOM	2813	CA	MET	B	31	-6.849	-38.064	-41.424	1.00	34.91	BBBB
ATOM	2821	CA	ALA	B	32	-6.510	-34.511	-42.722	1.00	37.55	BBBB
ATOM	2826	CA	GLN	B	33	-5.182	-36.070	-45.938	1.00	38.24	BBBB
ATOM	2835	CA	GLY	B	34	-8.305	-38.169	-46.353	1.00	35.75	BBBB
ATOM	2839	CA	TRP	B	35	-7.016	-41.246	-44.508	1.00	34.58	BBBB
ATOM	2853	CA	GLN	B	36	-9.175	-43.535	-42.402	1.00	35.40	BBBB
ATOM	2862	CA	VAL	B	37	-7.417	-44.516	-39.184	1.00	34.16	BBBB
ATOM	2869	CA	ARG	B	38	-8.219	-47.286	-36.730	1.00	31.56	BBBB
ATOM	2880	CA	TRP	B	39	-6.456	-48.070	-33.471	1.00	27.41	BBBB
ATOM	2894	CA	LEU	B	40	-5.200	-51.364	-32.026	1.00	24.71	BBBB
ATOM	2902	CA	GLY	B	41	-4.691	-51.450	-28.257	1.00	23.47	BBBB
ATOM	2906	CA	THR	B	42	-5.787	-53.141	-25.027	1.00	29.84	BBBB
ATOM	2913	CA	ALA	B	43	-9.000	-52.595	-23.047	1.00	38.81	BBBB
ATOM	2918	CA	ASP	B	44	-7.455	-51.942	-19.632	1.00	44.47	BBBB
ATOM	2926	CA	ARG	B	45	-4.887	-49.367	-20.763	1.00	40.44	BBBB
ATOM	2937	CA	MET	B	46	-4.881	-45.581	-21.249	1.00	36.33	BBBB
ATOM	2945	CA	GLU	B	47	-5.458	-45.655	-25.029	1.00	31.79	BBBB
ATOM	2954	CA	ALA	B	48	-8.821	-47.344	-24.414	1.00	32.58	BBBB
ATOM	2959	CA	ASP	B	49	-10.143	-44.065	-23.009	1.00	35.60	BBBB
ATOM	2967	CA	LEU	B	50	-8.026	-41.484	-24.840	1.00	33.49	BBBB
ATOM	2975	CA	VAL	B	51	-8.299	-42.641	-28.449	1.00	32.68	BBBB
ATOM	2983	CA	PRO	B	52	-12.111	-42.601	-28.453	1.00	34.43	BBBB
ATOM	2989	CA	LYS	B	53	-11.998	-39.054	-27.064	1.00	36.73	BBBB
ATOM	2998	CA	HIS	B	54	-10.116	-38.212	-30.259	1.00	34.62	BBBB
ATOM	3008	CA	GLY	B	55	-12.938	-39.481	-32.447	1.00	35.34	BBBB
ATOM	3012	CA	ILE	B	56	-10.909	-42.517	-33.514	1.00	33.81	BBBB
ATOM	3020	CA	GLU	B	57	-12.228	-46.083	-33.467	1.00	34.16	BBBB
ATOM	3029	CA	ILE	B	58	-10.217	-48.658	-31.553	1.00	31.38	BBBB
ATOM	3037	CA	ASP	B	59	-10.039	-52.442	-31.720	1.00	31.09	BBBB
ATOM	3045	CA	PHE	B	60	-8.809	-54.410	-28.713	1.00	30.32	BBBB
ATOM	3056	CA	ILE	B	61	-6.832	-57.616	-28.269	1.00	28.55	BBBB
ATOM	3064	CA	ARG	B	62	-5.709	-59.416	-25.133	1.00	30.76	BBBB
ATOM	3075	CA	ILE	B	63	-2.036	-59.770	-24.231	1.00	31.38	BBBB
ATOM	3083	CA	SER	B	64	-2.356	-60.520	-20.505	1.00	37.51	BBBB
ATOM	3089	CA	GLY	B	65	0.679	-62.355	-19.199	1.00	37.13	BBBB
ATOM	3093	CA	LEU	B	66	2.591	-61.413	-22.355	1.00	33.17	BBBB
ATOM	3101	CA	ARG	B	67	3.671	-57.928	-21.277	1.00	30.90	BBBB

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ATOM   3112  CA  GLY B  68       7.380 -57.427 -20.685  1.00 26.79 BBBB
ATOM   3116  CA  LYS B  69       8.238 -60.463 -22.796  1.00 23.93 BBBB
ATOM   3125  CA  GLY B  70      10.755 -60.229 -25.636  1.00 22.26 BBBB
ATOM   3129  CA  ILE B  71      10.357 -62.386 -28.762  1.00 23.55 BBBB
ATOM   3137  CA  LYS B  72      12.038 -65.491 -27.343  1.00 24.92 BBBB
ATOM   3146  CA  ALA B  73       9.839 -65.306 -24.233  1.00 21.18 BBBB
ATOM   3151  CA  LEU B  74       6.745 -64.762 -26.387  1.00 19.36 BBBB
ATOM   3159  CA  ILE B  75       7.434 -67.768 -28.601  1.00 21.18 BBBB
ATOM   3167  CA  ALA B  76       7.996 -69.726 -25.374  1.00 21.72 BBBB
ATOM   3172  CA  ALA B  77       4.289 -69.121 -24.655  1.00 21.07 BBBB
ATOM   3178  CA  PRO B  78       2.772 -70.846 -27.771  1.00 20.95 BBBB
ATOM   3184  CA  LEU B  79      -0.896 -70.728 -26.783  1.00 21.32 BBBB
ATOM   3192  CA  ARG B  80      -0.980 -67.115 -25.637  1.00 21.30 BBBB
ATOM   3203  CA  ILE B  81       1.113 -65.621 -28.421  1.00 19.47 BBBB
ATOM   3211  CA  PHE B  82      -0.875 -67.582 -31.038  1.00 19.15 BBBB
ATOM   3222  CA  ASN B  83      -4.150 -66.332 -29.577  1.00 20.90 BBBB
ATOM   3230  CA  ALA B  84      -3.177 -62.647 -29.484  1.00 19.30 BBBB
ATOM   3235  CA  TRP B  85      -1.820 -63.111 -33.032  1.00 20.56 BBBB
ATOM   3249  CA  ARG B  86      -5.140 -64.660 -34.166  1.00 23.28 BBBB
ATOM   3260  CA  GLN B  87      -7.101 -61.802 -32.567  1.00 24.07 BBBB
ATOM   3269  CA  ALA B  88      -4.996 -59.183 -34.355  1.00 23.78 BBBB
ATOM   3274  CA  ARG B  89      -5.285 -61.111 -37.636  1.00 24.94 BBBB
ATOM   3285  CA  ALA B  90      -9.088 -61.151 -37.383  1.00 26.16 BBBB
ATOM   3290  CA  ILE B  91      -9.108 -57.400 -36.733  1.00 26.97 BBBB
ATOM   3298  CA  MET B  92      -6.872 -56.693 -39.717  1.00 29.03 BBBB
ATOM   3306  CA  LYS B  93      -8.735 -59.038 -42.050  1.00 33.20 BBBB
ATOM   3315  CA  ALA B  94     -11.943 -57.157 -41.183  1.00 33.62 BBBB
ATOM   3320  CA  TYR B  95     -10.504 -53.620 -41.224  1.00 33.83 BBBB
ATOM   3332  CA  LYS B  96      -8.104 -54.327 -44.122  1.00 33.85 BBBB
ATOM   3342  CA  PRO B  97      -5.490 -51.623 -43.419  1.00 31.82 BBBB
ATOM   3348  CA  ASP B  98      -3.049 -50.685 -46.188  1.00 29.78 BBBB
ATOM   3356  CA  VAL B  99      -0.296 -50.214 -43.660  1.00 26.75 BBBB
ATOM   3363  CA  VAL B 100       0.227 -50.613 -39.936  1.00 23.59 BBBB
ATOM   3370  CA  LEU B 101       2.214 -48.199 -37.797  1.00 21.59 BBBB
ATOM   3378  CA  GLY B 102       3.796 -49.357 -34.549  1.00 19.23 BBBB
ATOM   3382  CA  MET B 103       4.892 -46.597 -32.191  1.00 18.93 BBBB
ATOM   3390  CA  GLY B 104       6.275 -49.080 -29.686  1.00 21.89 BBBB
ATOM   3394  CA  GLY B 105       4.593 -50.905 -26.827  1.00 23.54 BBBB
ATOM   3398  CA  TYR B 106       3.818 -54.554 -26.159  1.00 22.37 BBBB
ATOM   3410  CA  VAL B 107       0.557 -54.694 -28.099  1.00 18.06 BBBB
ATOM   3417  CA  SER B 108       2.488 -53.892 -31.290  1.00 19.67 BBBB
ATOM   3423  CA  GLY B 109       4.251 -57.256 -31.023  1.00 20.03 BBBB
ATOM   3428  CA  PRO B 110       1.251 -59.478 -31.855  1.00 18.99 BBBB
ATOM   3434  CA  GLY B 111      -0.160 -56.702 -34.025  1.00 19.60 BBBB
ATOM   3438  CA  GLY B 112       3.014 -56.417 -36.074  1.00 19.97 BBBB
ATOM   3442  CA  LEU B 113       3.265 -60.184 -36.429  1.00 19.49 BBBB
ATOM   3450  CA  ALA B 114      -0.334 -60.292 -37.661  1.00 18.70 BBBB
ATOM   3455  CA  ALA B 115       0.167 -57.516 -40.229  1.00 21.84 BBBB
ATOM   3460  CA  TRP B 116       3.365 -59.126 -41.478  1.00 23.22 BBBB
ATOM   3474  CA  SER B 117       1.735 -62.573 -41.873  1.00 22.61 BBBB
ATOM   3480  CA  LEU B 118      -1.069 -60.957 -43.882  1.00 25.70 BBBB
ATOM   3488  CA  GLY B 119       1.354 -59.174 -46.192  1.00 27.80 BBBB
ATOM   3492  CA  ILE B 120       0.568 -55.744 -44.731  1.00 24.85 BBBB
ATOM   3501  CA  PRO B 121       3.625 -53.477 -44.591  1.00 22.63 BBBB
ATOM   3507  CA  VAL B 122       4.743 -52.594 -41.083  1.00 22.03 BBBB
ATOM   3514  CA  VAL B 123       6.200 -49.184 -40.310  1.00 20.82 BBBB
ATOM   3521  CA  LEU B 124       7.749 -48.485 -36.915  1.00 22.10 BBBB
ATOM   3529  CA  HIS B 125       8.814 -45.413 -34.981  1.00 21.42 BBBB
ATOM   3539  CA  GLU B 126      10.947 -45.452 -31.817  1.00 22.15 BBBB
ATOM   3548  CA  GLN B 127      10.682 -42.270 -29.735  1.00 22.81 BBBB
ATOM   3557  CA  ASN B 128      13.406 -43.097 -27.216  1.00 22.96 BBBB
ATOM   3565  CA  GLY B 129      17.203 -43.019 -27.294  1.00 25.36 BBBB
ATOM   3569  CA  ILE B 130      17.160 -46.716 -26.488  1.00 28.00 BBBB
ATOM   3577  CA  ALA B 131      14.978 -49.139 -28.461  1.00 25.88 BBBB
ATOM   3582  CA  GLY B 132      12.007 -50.532 -26.568  1.00 24.05 BBBB
ATOM   3586  CA  LEU B 133      11.903 -54.293 -26.020  1.00 24.54 BBBB
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ATOM   3594  CA  THR B 134       9.202 -54.860 -28.639  1.00 21.22 BBBB
ATOM   3601  CA  ASN B 135      10.407 -52.419 -31.324  1.00 20.50 BBBB
ATOM   3609  CA  LYS B 136      13.886 -53.949 -31.144  1.00 22.79 BBBB
ATOM   3618  CA  TRP B 137      12.753 -57.345 -32.424  1.00 22.06 BBBB
ATOM   3632  CA  LEU B 138       9.744 -56.188 -34.431  1.00 23.15 BBBB
ATOM   3640  CA  ALA B 139      12.128 -54.092 -36.542  1.00 25.29 BBBB
ATOM   3645  CA  LYS B 140      13.279 -57.337 -38.182  1.00 28.05 BBBB
ATOM   3654  CA  ILE B 141       9.963 -57.818 -40.016  1.00 26.09 BBBB
ATOM   3662  CA  ALA B 142       9.331 -54.107 -40.498  1.00 25.03 BBBB
ATOM   3667  CA  THR B 143       9.262 -52.595 -43.984  1.00 26.10 BBBB
ATOM   3674  CA  LYS B 144      10.436 -49.238 -42.618  1.00 24.73 BBBB
ATOM   3683  CA  VAL B 145      11.947 -48.311 -39.252  1.00 23.62 BBBB
ATOM   3690  CA  MET B 146      12.338 -44.736 -37.993  1.00 23.15 BBBB
ATOM   3698  CA  GLN B 147      13.762 -43.418 -34.712  1.00 25.05 BBBB
ATOM   3707  CA  ALA B 148      13.559 -40.032 -33.009  1.00 26.88 BBBB
ATOM   3712  CA  PHE B 149      17.239 -39.820 -32.098  1.00 29.39 BBBB
ATOM   3724  CA  PRO B 150      20.310 -41.541 -33.535  1.00 31.87 BBBB
ATOM   3730  CA  GLY B 151      21.629 -44.537 -31.595  1.00 32.62 BBBB
ATOM   3734  CA  ALA B 152      18.447 -46.476 -30.753  1.00 32.71 BBBB
ATOM   3739  CA  PHE B 153      18.925 -48.506 -33.937  1.00 34.83 BBBB
ATOM   3751  CA  PRO B 154      22.158 -48.751 -35.993  1.00 38.97 BBBB
ATOM   3757  CA  ASN B 155      20.765 -47.568 -39.346  1.00 41.08 BBBB
ATOM   3765  CA  ALA B 156      17.170 -46.407 -38.843  1.00 37.55 BBBB
ATOM   3770  CA  GLU B 157      16.367 -43.044 -40.460  1.00 34.40 BBBB
ATOM   3779  CA  VAL B 158      16.337 -40.344 -37.764  1.00 31.16 BBBB
ATOM   3786  CA  VAL B 159      13.155 -38.265 -37.889  1.00 28.10 BBBB
ATOM   3793  CA  GLY B 160      12.724 -36.921 -34.355  1.00 26.93 BBBB
ATOM   3797  CA  ASN B 161       9.456 -36.807 -32.375  1.00 25.27 BBBB
ATOM   3806  CA  PRO B 162       6.315 -34.747 -33.004  1.00 26.14 BBBB
ATOM   3812  CA  VAL B 163       6.456 -31.379 -31.216  1.00 27.75 BBBB
ATOM   3819  CA  ARG B 164       3.667 -28.953 -30.246  1.00 32.36 BBBB
ATOM   3830  CA  THR B 165       3.038 -26.307 -32.924  1.00 31.74 BBBB
ATOM   3837  CA  ASP B 166       3.252 -23.404 -30.466  1.00 30.64 BBBB
ATOM   3845  CA  VAL B 167       6.746 -24.503 -29.440  1.00 25.91 BBBB
ATOM   3852  CA  LEU B 168       7.780 -25.002 -33.075  1.00 28.46 BBBB
ATOM   3860  CA  ALA B 169       6.580 -21.455 -33.756  1.00 31.43 BBBB
ATOM   3865  CA  LEU B 170       9.002 -19.905 -31.268  1.00 29.60 BBBB
ATOM   3874  CA  PRO B 171      11.611 -17.457 -32.642  1.00 30.11 BBBB
ATOM   3880  CA  LEU B 172      15.157 -18.780 -33.062  1.00 28.33 BBBB
ATOM   3889  CA  PRO B 173      17.450 -18.550 -29.977  1.00 25.25 BBBB
ATOM   3895  CA  GLN B 174      19.526 -15.527 -31.049  1.00 25.46 BBBB
ATOM   3904  CA  GLN B 175      16.365 -13.525 -31.718  1.00 28.47 BBBB
ATOM   3913  CA  ARG B 176      14.611 -14.635 -28.525  1.00 29.01 BBBB
ATOM   3924  CA  LEU B 177      17.673 -13.970 -26.331  1.00 29.90 BBBB
ATOM   3932  CA  ALA B 178      18.766 -10.776 -28.131  1.00 30.78 BBBB
ATOM   3937  CA  GLY B 179      19.846  -7.993 -25.784  1.00 30.10 BBBB
ATOM   3941  CA  ARG B 180      18.676  -9.965 -22.787  1.00 28.97 BBBB
ATOM   3952  CA  GLU B 181      20.545  -9.027 -19.621  1.00 31.79 BBBB
ATOM   3961  CA  GLY B 182      19.871  -9.586 -15.943  1.00 27.75 BBBB
ATOM   3966  CA  PRO B 183      19.450 -12.832 -13.913  1.00 22.93 BBBB
ATOM   3972  CA  VAL B 184      19.524 -16.146 -15.729  1.00 18.01 BBBB
ATOM   3979  CA  ARG B 185      15.873 -17.216 -16.011  1.00 17.62 BBBB
ATOM   3990  CA  VAL B 186      15.508 -20.771 -14.741  1.00 16.47 BBBB
ATOM   3997  CA  LEU B 187      12.361 -22.710 -15.604  1.00 16.75 BBBB
ATOM   4005  CA  VAL B 188      11.774 -25.775 -13.381  1.00 18.41 BBBB
ATOM   4012  CA  VAL B 189       9.298 -28.234 -14.948  1.00 22.11 BBBB
ATOM   4019  CA  GLY B 190       7.914 -31.188 -12.994  1.00 27.28 BBBB
ATOM   4023  CA  GLY B 191       4.935 -32.163 -15.115  1.00 31.94 BBBB
ATOM   4027  CA  SER B 192       1.313 -32.665 -14.064  1.00 35.91 BBBB
ATOM   4033  CA  GLN B 193       2.292 -34.763 -11.033  1.00 38.53 BBBB
ATOM   4042  CA  GLY B 194       5.398 -32.711 -10.350  1.00 35.02 BBBB
ATOM   4046  CA  ALA B 195       8.977 -33.819  -9.709  1.00 33.12 BBBB
ATOM   4051  CA  ARG B 196       9.538 -34.512  -6.010  1.00 32.63 BBBB
ATOM   4062  CA  ILE B 197      13.329 -34.168  -6.164  1.00 28.10 BBBB
ATOM   4070  CA  LEU B 198      13.069 -30.833  -8.003  1.00 26.58 BBBB
ATOM   4078  CA  ASN B 199      10.497 -29.447  -5.563  1.00 27.07 BBBB
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ATOM   4086  CA  GLN B 200      12.955 -30.326  -2.794  1.00 30.10 BBBB
ATOM   4095  CA  THR B 201      16.215 -29.345  -4.474  1.00 27.34 BBBB
ATOM   4102  CA  MET B 202      15.567 -26.048  -6.268  1.00 23.68 BBBB
ATOM   4111  CA  PRO B 203      14.608 -23.963  -3.220  1.00 23.84 BBBB
ATOM   4117  CA  GLN B 204      18.033 -24.708  -1.684  1.00 26.34 BBBB
ATOM   4126  CA  VAL B 205      19.672 -24.033  -5.043  1.00 24.44 BBBB
ATOM   4133  CA  ALA B 206      17.980 -20.610  -5.013  1.00 22.84 BBBB
ATOM   4138  CA  ALA B 207      19.442 -19.857  -1.576  1.00 26.65 BBBB
ATOM   4143  CA  LYS B 208      22.915 -20.595  -2.919  1.00 28.31 BBBB
ATOM   4152  CA  LEU B 209      22.577 -18.640  -6.171  1.00 25.68 BBBB
ATOM   4160  CA  GLY B 210      20.675 -15.628  -4.804  1.00 26.56 BBBB
ATOM   4164  CA  ASP B 211      20.370 -12.647  -7.190  1.00 28.28 BBBB
ATOM   4172  CA  SER B 212      22.098 -14.474 -10.067  1.00 25.73 BBBB
ATOM   4178  CA  VAL B 213      18.925 -16.308 -11.116  1.00 20.76 BBBB
ATOM   4185  CA  THR B 214      15.204 -15.726 -11.337  1.00 19.60 BBBB
ATOM   4192  CA  ILE B 215      13.076 -18.850 -11.169  1.00 18.75 BBBB
ATOM   4200  CA  TRP B 216       9.661 -19.973 -12.378  1.00 19.34 BBBB
ATOM   4214  CA  HIS B 217       9.015 -23.303 -10.680  1.00 21.06 BBBB
ATOM   4224  CA  GLN B 218       6.149 -25.594 -11.735  1.00 24.30 BBBB
ATOM   4233  CA  SER B 219       5.463 -27.800  -8.684  1.00 26.73 BBBB
ATOM   4239  CA  GLY B 220       2.855 -30.242  -9.961  1.00 30.53 BBBB
ATOM   4243  CA  LYS B 221      -0.657 -30.914  -8.628  1.00 35.12 BBBB
ATOM   4252  CA  GLY B 222      -1.195 -29.899  -5.011  1.00 35.34 BBBB
ATOM   4256  CA  SER B 223       2.451 -28.934  -4.418  1.00 33.98 BBBB
ATOM   4262  CA  GLN B 224       2.187 -25.208  -5.186  1.00 33.71 BBBB
ATOM   4271  CA  GLN B 225       1.823 -24.239  -1.519  1.00 32.32 BBBB
ATOM   4280  CA  SER B 226       4.701 -26.309  -0.122  1.00 28.30 BBBB
ATOM   4286  CA  VAL B 227       7.214 -25.247  -2.791  1.00 24.28 BBBB
ATOM   4293  CA  GLU B 228       6.178 -21.592  -2.387  1.00 27.23 BBBB
ATOM   4302  CA  GLN B 229       6.853 -22.046   1.329  1.00 28.38 BBBB
ATOM   4311  CA  ALA B 230      10.185 -23.754   0.682  1.00 26.18 BBBB
ATOM   4316  CA  TYR B 231      11.371 -20.766  -1.366  1.00 25.47 BBBB
ATOM   4328  CA  ALA B 232      10.342 -18.322   1.368  1.00 27.51 BBBB
ATOM   4333  CA  GLU B 233      12.145 -20.441   3.966  1.00 30.87 BBBB
ATOM   4342  CA  ALA B 234      15.215 -20.417   1.714  1.00 28.48 BBBB
ATOM   4347  CA  GLY B 235      15.033 -16.627   1.815  1.00 26.23 BBBB
ATOM   4351  CA  GLN B 236      14.121 -16.198  -1.870  1.00 25.53 BBBB
ATOM   4361  CA  PRO B 237      10.336 -15.587  -1.720  1.00 24.65 BBBB
ATOM   4367  CA  GLN B 238      10.277 -13.558  -4.945  1.00 24.29 BBBB
ATOM   4376  CA  HIS B 239      10.526 -16.608  -7.201  1.00 22.08 BBBB
ATOM   4386  CA  LYS B 240       7.375 -17.589  -9.105  1.00 23.26 BBBB
ATOM   4395  CA  VAL B 241       5.740 -20.911  -8.277  1.00 23.78 BBBB
ATOM   4402  CA  THR B 242       2.758 -22.301 -10.177  1.00 25.93 BBBB
ATOM   4409  CA  GLU B 243       0.999 -25.651  -9.837  1.00 27.03 BBBB
ATOM   4418  CA  PHE B 244       0.964 -26.068 -13.620  1.00 26.54 BBBB
ATOM   4429  CA  ILE B 245       1.932 -24.242 -16.802  1.00 28.48 BBBB
ATOM   4437  CA  ASP B 246      -0.754 -24.396 -19.457  1.00 36.00 BBBB
ATOM   4445  CA  ASP B 247       1.245 -22.392 -21.999  1.00 30.74 BBBB
ATOM   4453  CA  MET B 248       4.625 -24.136 -22.138  1.00 28.41 BBBB
ATOM   4461  CA  ALA B 249       5.512 -22.216 -25.290  1.00 24.67 BBBB
ATOM   4466  CA  ALA B 250       5.188 -18.933 -23.390  1.00 21.78 BBBB
ATOM   4471  CA  ALA B 251       7.301 -20.259 -20.501  1.00 20.85 BBBB
ATOM   4476  CA  TYR B 252       9.972 -21.616 -22.886  1.00 22.78 BBBB
ATOM   4488  CA  ALA B 253      10.131 -18.224 -24.636  1.00 23.54 BBBB
ATOM   4493  CA  TRP B 254      10.829 -16.534 -21.303  1.00 19.76 BBBB
ATOM   4507  CA  ALA B 255      13.399 -19.025 -20.003  1.00 19.51 BBBB
ATOM   4512  CA  ASP B 256      17.176 -19.026 -20.434  1.00 17.58 BBBB
ATOM   4520  CA  VAL B 257      17.535 -22.603 -19.194  1.00 18.53 BBBB
ATOM   4527  CA  VAL B 258      15.208 -25.456 -18.234  1.00 19.32 BBBB
ATOM   4534  CA  VAL B 259      15.581 -27.957 -15.374  1.00 19.85 BBBB
ATOM   4541  CA  CYS B 260      13.454 -31.055 -15.946  1.00 22.00 BBBB
ATOM   4547  CA  ARG B 261      13.170 -34.800 -16.515  1.00 23.75 BBBB
ATOM   4558  CA  SER B 262      13.975 -36.189 -19.948  1.00 23.18 BBBB
ATOM   4564  CA  GLY B 263      11.026 -38.079 -21.361  1.00 22.85 BBBB
ATOM   4568  CA  ALA B 264      11.482 -38.564 -25.115  1.00 24.25 BBBB
ATOM   4573  CA  LEU B 265       8.846 -36.037 -26.205  1.00 24.66 BBBB
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ATOM   4581  CA  THR B 266      10.194 -33.557 -23.657  1.00 22.34 BBBB
ATOM   4588  CA  VAL B 267      13.730 -33.762 -25.023  1.00 21.11 BBBB
ATOM   4595  CA  SER B 268      12.411 -33.191 -28.567  1.00 21.96 BBBB
ATOM   4601  CA  GLU B 269      10.282 -30.272 -27.378  1.00 21.95 BBBB
ATOM   4610  CA  ILE B 270      13.295 -28.698 -25.638  1.00 20.62 BBBB
ATOM   4618  CA  ALA B 271      15.440 -29.058 -28.776  1.00 22.45 BBBB
ATOM   4623  CA  ALA B 272      12.719 -27.451 -30.898  1.00 22.17 BBBB
ATOM   4628  CA  ALA B 273      12.361 -24.596 -28.407  1.00 21.97 BBBB
ATOM   4633  CA  GLY B 274      16.093 -24.023 -28.709  1.00 21.07 BBBB
ATOM   4637  CA  LEU B 275      16.666 -24.057 -24.966  1.00 19.78 BBBB
ATOM   4646  CA  PRO B 276      19.651 -25.199 -22.875  1.00 16.62 BBBB
ATOM   4652  CA  ALA B 277      18.638 -27.807 -20.321  1.00 15.80 BBBB
ATOM   4657  CA  LEU B 278      19.896 -29.429 -17.145  1.00 18.48 BBBB
ATOM   4665  CA  PHE B 279      18.266 -32.838 -17.392  1.00 21.59 BBBB
ATOM   4676  CA  VAL B 280      17.502 -34.902 -14.281  1.00 25.67 BBBB
ATOM   4684  CA  PRO B 281      16.698 -38.320 -15.824  1.00 29.05 BBBB
ATOM   4690  CA  PHE B 282      14.246 -40.496 -13.926  1.00 37.13 BBBB
ATOM   4701  CA  GLN B 283      16.319 -43.395 -12.591  1.00 41.11 BBBB
ATOM   4710  CA  HIS B 284      15.641 -46.917 -13.843  1.00 43.69 BBBB
ATOM   4720  CA  LYS B 285      17.767 -49.993 -14.571  1.00 45.34 BBBB
ATOM   4729  CA  ASP B 286      16.949 -49.299 -18.222  1.00 43.26 BBBB
ATOM   4737  CA  ARG B 287      17.951 -45.623 -17.883  1.00 36.28 BBBB
ATOM   4748  CA  GLN B 288      15.622 -44.804 -20.755  1.00 30.77 BBBB
ATOM   4757  CA  GLN B 289      15.474 -41.099 -19.904  1.00 29.46 BBBB
ATOM   4766  CA  TYR B 290      19.228 -40.984 -19.550  1.00 29.55 BBBB
ATOM   4778  CA  TRP B 291      19.542 -42.282 -23.116  1.00 28.07 BBBB
ATOM   4792  CA  ASN B 292      16.902 -39.784 -24.270  1.00 26.06 BBBB
ATOM   4800  CA  ALA B 293      18.926 -36.822 -22.979  1.00 25.69 BBBB
ATOM   4805  CA  LEU B 294      22.354 -38.088 -24.032  1.00 25.90 BBBB
ATOM   4814  CA  PRO B 295      21.998 -36.870 -27.635  1.00 26.15 BBBB
ATOM   4820  CA  LEU B 296      21.521 -33.265 -26.481  1.00 25.42 BBBB
ATOM   4828  CA  GLU B 297      24.354 -33.530 -23.953  1.00 28.78 BBBB
ATOM   4837  CA  LYS B 298      26.644 -34.947 -26.648  1.00 31.90 BBBB
ATOM   4846  CA  ALA B 299      25.773 -31.965 -28.847  1.00 30.38 BBBB
ATOM   4851  CA  GLY B 300      26.777 -29.635 -26.017  1.00 26.18 BBBB
ATOM   4855  CA  ALA B 301      23.214 -28.333 -25.638  1.00 22.50 BBBB
ATOM   4860  CA  ALA B 302      22.516 -29.770 -22.186  1.00 21.78 BBBB
ATOM   4865  CA  LYS B 303      23.979 -31.340 -19.048  1.00 25.86 BBBB
ATOM   4874  CA  ILE B 304      22.753 -34.598 -17.550  1.00 27.17 BBBB
ATOM   4882  CA  ILE B 305      22.843 -35.178 -13.813  1.00 29.01 BBBB
ATOM   4890  CA  GLU B 306      21.664 -38.702 -13.061  1.00 34.65 BBBB
ATOM   4899  CA  GLN B 307      20.377 -39.599  -9.613  1.00 40.54 BBBB
ATOM   4909  CA  PRO B 308      23.828 -40.891  -8.484  1.00 43.20 BBBB
ATOM   4915  CA  GLN B 309      25.247 -37.361  -8.787  1.00 43.46 BBBB
ATOM   4924  CA  LEU B 310      22.232 -35.166  -8.022  1.00 39.65 BBBB
ATOM   4932  CA  SER B 311      22.660 -32.714  -5.154  1.00 34.90 BBBB
ATOM   4938  CA  VAL B 312      21.990 -29.074  -4.341  1.00 31.50 BBBB
ATOM   4945  CA  ASP B 313      25.642 -28.202  -4.957  1.00 29.61 BBBB
ATOM   4953  CA  ALA B 314      25.782 -30.099  -8.254  1.00 26.47 BBBB
ATOM   4958  CA  VAL B 315      22.755 -28.215  -9.612  1.00 25.33 BBBB
ATOM   4965  CA  ALA B 316      23.888 -24.872  -8.199  1.00 27.13 BBBB
ATOM   4970  CA  ASN B 317      27.444 -25.246  -9.518  1.00 28.52 BBBB
ATOM   4978  CA  THR B 318      26.174 -26.371 -12.906  1.00 27.04 BBBB
ATOM   4985  CA  LEU B 319      23.883 -23.370 -13.357  1.00 25.21 BBBB
ATOM   4993  CA  ALA B 320      26.445 -20.931 -11.957  1.00 24.59 BBBB
ATOM   4998  CA  GLY B 321      28.934 -22.031 -14.591  1.00 24.34 BBBB
ATOM   5002  CA  TRP B 322      26.738 -21.007 -17.521  1.00 21.72 BBBB
ATOM   5016  CA  SER B 323      27.141 -17.404 -18.692  1.00 19.04 BBBB
ATOM   5022  CA  ARG B 324      24.725 -15.741 -21.112  1.00 18.09 BBBB
ATOM   5033  CA  GLU B 325      27.220 -16.368 -23.954  1.00 16.96 BBBB
ATOM   5042  CA  THR B 326      27.460 -20.055 -23.070  1.00 16.39 BBBB
ATOM   5049  CA  LEU B 327      23.659 -20.305 -22.780  1.00 17.27 BBBB
ATOM   5057  CA  LEU B 328      23.175 -18.745 -26.222  1.00 17.39 BBBB
ATOM   5065  CA  THR B 329      25.567 -21.335 -27.688  1.00 21.30 BBBB
ATOM   5072  CA  MET B 330      23.771 -24.153 -25.870  1.00 19.91 BBBB
ATOM   5080  CA  ALA B 331      20.412 -22.871 -27.098  1.00 18.49 BBBB
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ATOM   5085  CA  GLU B 332      21.626 -22.827 -30.704  1.00 21.47 BBBB
ATOM   5094  CA  ARG B 333      23.040 -26.330 -30.408  1.00 23.77 BBBB
ATOM   5105  CA  ALA B 334      19.648 -27.420 -29.063  1.00 22.88 BBBB
ATOM   5110  CA  ARG B 335      17.795 -25.892 -32.002  1.00 23.54 BBBB
ATOM   5121  CA  ALA B 336      20.330 -27.477 -34.372  1.00 26.85 BBBB
ATOM   5126  CA  ALA B 337      19.740 -30.925 -32.865  1.00 30.89 BBBB
ATOM   5131  CA  SER B 338      16.008 -30.432 -33.408  1.00 32.41 BBBB
ATOM   5137  CA  ILE B 339      13.882 -31.941 -36.187  1.00 34.35 BBBB
ATOM   5146  CA  PRO B 340      10.733 -29.730 -36.600  1.00 34.94 BBBB
ATOM   5152  CA  ASP B 341       8.711 -31.820 -39.056  1.00 33.33 BBBB
ATOM   5160  CA  ALA B 342       8.875 -35.238 -37.411  1.00 29.09 BBBB
ATOM   5165  CA  THR B 343       5.115 -35.696 -37.744  1.00 28.55 BBBB
ATOM   5172  CA  GLU B 344       5.085 -34.933 -41.480  1.00 32.00 BBBB
ATOM   5181  CA  ARG B 345       8.138 -37.123 -42.067  1.00 31.44 BBBB
ATOM   5192  CA  VAL B 346       6.578 -40.151 -40.384  1.00 28.61 BBBB
ATOM   5199  CA  ALA B 347       3.249 -39.617 -42.137  1.00 28.96 BBBB
ATOM   5204  CA  ASN B 348       5.035 -39.286 -45.493  1.00 34.56 BBBB
ATOM   5212  CA  GLU B 349       6.954 -42.540 -44.956  1.00 34.86 BBBB
ATOM   5221  CA  VAL B 350       3.767 -44.306 -43.919  1.00 33.79 BBBB
ATOM   5228  CA  SER B 351       2.196 -42.946 -47.095  1.00 36.67 BBBB
ATOM   5234  CA  ARG B 352       5.114 -44.088 -49.251  1.00 40.03 BBBB
ATOM   5245  CA  VAL B 353       5.089 -47.587 -47.737  1.00 42.78 BBBB
ATOM   5252  CA  ALA B 354       1.336 -47.957 -48.212  1.00 47.24 BBBB
ATOM   5257  CA  ARG B 355       2.035 -46.964 -51.824  1.00 52.71 BBBB
ATOM   5268  CA  ALA B 356       4.453 -49.913 -51.809  1.00 54.93 BBBB
ATOM   5273  CA  LEU B 357       7.023 -47.522 -53.289  1.00 57.81 BBBB
END
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TABLE 3 ATOMIC COORDINATES OF E.COLI MURG C-ALPHA BACKBONE AND CONSERVED AMINO ACID RESIDUES

ATOM	2649	CA	LYS	B	7	-6.512	-45.403	-47.519	1.00	45.28	BBBB
ATOM	2651	CA	ARG	B	8	-6.682	-47.303	-44.240	1.00	38.63	BBBB
ATOM	2662	CA	LEU	B	9	-4.094	-47.039	-41.477	1.00	30.88	BBBB
ATOM	2670	CA	MET	B	10	-4.048	-49.055	-38.275	1.00	26.66	BBBB
ATOM	2678	CA	VAL	B	11	-1.982	-47.605	-35.449	1.00	23.16	BBBB
ATOM	2685	CA	MET	B	12	-0.523	-49.707	-32.613	1.00	24.54	BBBB
ATOM	2693	CA	ALA	B	13	0.508	-47.410	-29.752	1.00	29.43	BBBB
ATOM	2697	N	GLY	B	14	0.150	-47.934	-27.405	1.00	32.46	BBBB
ATOM	2698	CA	GLY	B	14	-0.513	-47.804	-26.120	1.00	33.82	BBBB
ATOM	2699	C	GLY	B	14	-0.107	-46.595	-25.299	1.00	34.82	BBBB
ATOM	2700	O	GLY	B	14	0.975	-46.040	-25.479	1.00	35.47	BBBB
ATOM	2701	N	GLY	B	15	-0.986	-46.188	-24.385	1.00	35.56	BBBB
ATOM	2702	CA	GLY	B	15	-0.700	-45.047	-23.536	1.00	36.08	BBBB
ATOM	2703	C	GLY	B	15	0.539	-45.254	-22.683	1.00	36.84	BBBB
ATOM	2704	O	GLY	B	15	1.293	-44.311	-22.426	1.00	36.03	BBBB
ATOM	2706	CA	THR	B	16	1.920	-46.787	-21.421	1.00	38.51	BBBB
ATOM	2713	CA	GLY	B	17	5.367	-45.567	-22.392	1.00	36.57	BBBB
ATOM	2716	N	GLY	B	18	3.949	-43.752	-23.150	1.00	33.83	BBBB
ATOM	2717	CA	GLY	B	18	3.631	-42.529	-23.872	1.00	33.48	BBBB
ATOM	2718	C	GLY	B	18	3.825	-42.593	-25.378	1.00	33.12	BBBB
ATOM	2719	O	GLY	B	18	4.345	-41.650	-25.984	1.00	35.38	BBBB
ATOM	2720	N	HIS	B	19	3.416	-43.699	-25.988	1.00	30.26	BBBB
ATOM	2721	CA	HIS	B	19	3.548	-43.865	-27.435	1.00	28.22	BBBB
ATOM	2722	CB	HIS	B	19	3.772	-45.349	-27.779	1.00	25.81	BBBB
ATOM	2723	CG	HIS	B	19	4.957	-45.966	-27.094	1.00	25.35	BBBB
ATOM	2724	CD2	HIS	B	19	6.281	-45.694	-27.184	1.00	24.18	BBBB
ATOM	2725	ND1	HIS	B	19	4.845	-47.025	-26.217	1.00	24.57	BBBB
ATOM	2726	CE1	HIS	B	19	6.046	-47.380	-25.798	1.00	23.08	BBBB
ATOM	2727	NE2	HIS	B	19	6.936	-46.589	-26.369	1.00	25.51	BBBB
ATOM	2728	C	HIS	B	19	2.280	-43.370	-28.144	1.00	27.91	BBBB
ATOM	2729	O	HIS	B	19	2.300	-43.049	-29.337	1.00	26.91	BBBB
ATOM	2731	CA	VAL	B	20	-0.098	-42.894	-27.965	1.00	27.77	BBBB
ATOM	2738	CA	PHE	B	21	0.517	-39.136	-28.160	1.00	29.00	BBBB
ATOM	2750	CA	PRO	B	22	2.986	-39.252	-31.086	1.00	26.12	BBBB
ATOM	2756	CA	GLY	B	23	0.787	-41.864	-32.752	1.00	25.07	BBBB
ATOM	2760	CA	LEU	B	24	-2.201	-39.551	-32.401	1.00	25.32	BBBB
ATOM	2768	CA	ALA	B	25	-0.197	-36.754	-34.013	1.00	25.94	BBBB
ATOM	2773	CA	VAL	B	26	0.466	-38.955	-37.056	1.00	25.70	BBBB
ATOM	2780	CA	ALA	B	27	-3.116	-40.222	-37.199	1.00	26.15	BBBB
ATOM	2785	CA	HIS	B	28	-4.574	-36.702	-37.190	1.00	29.32	BBBB
ATOM	2795	CA	HIS	B	29	-2.070	-35.623	-39.806	1.00	32.38	BBBB
ATOM	2805	CA	LEU	B	30	-3.136	-38.417	-42.162	1.00	32.00	BBBB
ATOM	2813	CA	MET	B	31	-6.849	-38.064	-41.424	1.00	34.91	BBBB
ATOM	2821	CA	ALA	B	32	-6.510	-34.511	-42.722	1.00	37.55	BBBB
ATOM	2826	CA	GLN	B	33	-5.182	-36.070	-45.938	1.00	38.24	BBBB
ATOM	2835	CA	GLY	B	34	-8.305	-38.169	-46.353	1.00	35.75	BBBB
ATOM	2839	CA	TRP	B	35	-7.016	-41.246	-44.508	1.00	34.58	BBBB
ATOM	2853	CA	GLN	B	36	-9.175	-43.535	-42.402	1.00	35.40	BBBB
ATOM	2862	CA	VAL	B	37	-7.417	-44.516	-39.184	1.00	34.16	BBBB
ATOM	2869	CA	ARG	B	38	-8.219	-47.286	-36.730	1.00	31.56	BBBB
ATOM	2880	CA	TRP	B	39	-6.456	-48.070	-33.471	1.00	27.41	BBBB
ATOM	2894	CA	LEU	B	40	-5.200	-51.364	-32.026	1.00	24.71	BBBB
ATOM	2902	CA	GLY	B	41	-4.691	-51.450	-28.257	1.00	23.47	BBBB
ATOM	2906	CA	THR	B	42	-5.787	-53.141	-25.027	1.00	29.84	BBBB
ATOM	2913	CA	ALA	B	43	-9.000	-52.595	-23.047	1.00	38.81	BBBB
ATOM	2918	CA	ASP	B	44	-7.455	-51.942	-19.632	1.00	44.47	BBBB
ATOM	2926	CA	ARG	B	45	-4.887	-49.367	-20.763	1.00	40.44	BBBB
ATOM	2937	CA	MET	B	46	-4.881	-45.581	-21.249	1.00	36.33	BBBB
ATOM	2945	CA	GLU	B	47	-5.458	-45.655	-25.029	1.00	31.79	BBBB
ATOM	2954	CA	ALA	B	48	-8.821	-47.344	-24.414	1.00	32.58	BBBB
ATOM	2959	CA	ASP	B	49	-10.143	-44.065	-23.009	1.00	35.60	BBBB

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ATOM   2967  CA  LEU B  50      -8.026 -41.484 -24.840  1.00 33.49 BBBB
ATOM   2975  CA  VAL B  51      -8.299 -42.641 -28.449  1.00 32.68 BBBB
ATOM   2983  CA  PRO B  52     -12.111 -42.601 -28.453  1.00 34.43 BBBB
ATOM   2989  CA  LYS B  53     -11.998 -39.054 -27.064  1.00 36.73 BBBB
ATOM   2998  CA  HIS B  54     -10.116 -38.212 -30.259  1.00 34.62 BBBB
ATOM   3008  CA  GLY B  55     -12.938 -39.481 -32.447  1.00 35.34 BBBB
ATOM   3012  CA  ILE B  56     -10.909 -42.517 -33.514  1.00 33.81 BBBB
ATOM   3020  CA  GLU B  57     -12.228 -46.083 -33.467  1.00 34.16 BBBB
ATOM   3029  CA  ILE B  58     -10.217 -48.658 -31.553  1.00 31.38 BBBB
ATOM   3037  CA  ASP B  59     -10.039 -52.442 -31.720  1.00 31.09 BBBB
ATOM   3045  CA  PHE B  60      -8.809 -54.410 -28.713  1.00 30.32 BBBB
ATOM   3056  CA  ILE B  61      -6.832 -57.616 -28.269  1.00 28.55 BBBB
ATOM   3064  CA  ARG B  62      -5.709 -59.416 -25.133  1.00 30.76 BBBB
ATOM   3075  CA  ILE B  63      -2.036 -59.770 -24.231  1.00 31.38 BBBB
ATOM   3083  CA  SER B  64      -2.356 -60.520 -20.505  1.00 37.51 BBBB
ATOM   3089  CA  GLY B  65       0.679 -62.355 -19.199  1.00 37.13 BBBB
ATOM   3093  CA  LEU B  66       2.591 -61.413 -22.355  1.00 33.17 BBBB
ATOM   3101  CA  ARG B  67       3.671 -57.928 -21.277  1.00 30.90 BBBB
ATOM   3112  CA  GLY B  68       7.380 -57.427 -20.685  1.00 26.79 BBBB
ATOM   3116  CA  LYS B  69       8.238 -60.463 -22.796  1.00 23.93 BBBB
ATOM   3125  CA  GLY B  70      10.755 -60.229 -25.636  1.00 22.26 BBBB
ATOM   3129  CA  ILE B  71      10.357 -62.386 -28.762  1.00 23.55 BBBB
ATOM   3137  CA  LYS B  72      12.038 -65.491 -27.343  1.00 24.92 BBBB
ATOM   3146  CA  ALA B  73       9.839 -65.306 -24.233  1.00 21.18 BBBB
ATOM   3151  CA  LEU B  74       6.745 -64.762 -26.387  1.00 19.36 BBBB
ATOM   3159  CA  ILE B  75       7.434 -67.768 -28.601  1.00 21.18 BBBB
ATOM   3167  CA  ALA B  76       7.996 -69.726 -25.374  1.00 21.72 BBBB
ATOM   3172  CA  ALA B  77       4.289 -69.121 -24.655  1.00 21.07 BBBB
ATOM   3178  CA  PRO B  78       2.772 -70.846 -27.771  1.00 20.95 BBBB
ATOM   3184  CA  LEU B  79      -0.896 -70.728 -26.783  1.00 21.32 BBBB
ATOM   3192  CA  ARG B  80      -0.980 -67.115 -25.637  1.00 21.30 BBBB
ATOM   3203  CA  ILE B  81       1.113 -65.621 -28.421  1.00 19.47 BBBB
ATOM   3211  CA  PHE B  82      -0.875 -67.582 -31.038  1.00 19.15 BBBB
ATOM   3222  CA  ASN B  83      -4.150 -66.332 -29.577  1.00 20.90 BBBB
ATOM   3230  CA  ALA B  84      -3.177 -62.647 -29.484  1.00 19.30 BBBB
ATOM   3235  CA  TRP B  85      -1.820 -63.111 -33.032  1.00 20.56 BBBB
ATOM   3249  CA  ARG B  86      -5.140 -64.660 -34.166  1.00 23.28 BBBB
ATOM   3260  CA  GLN B  87      -7.101 -61.802 -32.567  1.00 24.07 BBBB
ATOM   3269  CA  ALA B  88      -4.996 -59.183 -34.355  1.00 23.78 BBBB
ATOM   3274  CA  ARG B  89      -5.285 -61.111 -37.636  1.00 24.94 BBBB
ATOM   3285  CA  ALA B  90      -9.088 -61.151 -37.383  1.00 26.16 BBBB
ATOM   3290  CA  ILE B  91      -9.108 -57.400 -36.733  1.00 26.97 BBBB
ATOM   3298  CA  MET B  92      -6.872 -56.693 -39.717  1.00 29.03 BBBB
ATOM   3306  CA  LYS B  93      -8.735 -59.038 -42.050  1.00 33.20 BBBB
ATOM   3315  CA  ALA B  94     -11.943 -57.157 -41.183  1.00 33.62 BBBB
ATOM   3320  CA  TYR B  95     -10.504 -53.620 -41.224  1.00 33.83 BBBB
ATOM   3332  CA  LYS B  96      -8.104 -54.327 -44.122  1.00 33.85 BBBB
ATOM   3342  CA  PRO B  97      -5.490 -51.623 -43.419  1.00 31.82 BBBB
ATOM   3348  CA  ASP B  98      -3.049 -50.685 -46.188  1.00 29.78 BBBB
ATOM   3356  CA  VAL B  99      -0.296 -50.214 -43.660  1.00 26.75 BBBB
ATOM   3363  CA  VAL B 100       0.227 -50.613 -39.936  1.00 23.59 BBBB
ATOM   3370  CA  LEU B 101       2.214 -48.199 -37.797  1.00 21.59 BBBB
ATOM   3378  CA  GLY B 102       3.796 -49.357 -34.549  1.00 19.23 BBBB
ATOM   3382  CA  MET B 103       4.892 -46.597 -32.191  1.00 18.93 BBBB
ATOM   3389  N   GLY B 104       5.640 -48.450 -30.827  1.00 21.56 BBBB
ATOM   3390  CA  GLY B 104       6.275 -49.080 -29.686  1.00 21.89 BBBB
ATOM   3391  C   GLY B 104       5.192 -49.614 -28.764  1.00 23.28 BBBB
ATOM   3392  O   GLY B 104       4.009 -49.353 -28.980  1.00 22.50 BBBB
ATOM   3394  CA  GLY B 105       4.593 -50.905 -26.827  1.00 23.54 BBBB
ATOM   3398  CA  TYR B 106       3.818 -54.554 -26.159  1.00 22.37 BBBB
ATOM   3410  CA  VAL B 107       0.557 -54.694 -28.099  1.00 18.06 BBBB
ATOM   3417  CA  SER B 108       2.488 -53.892 -31.290  1.00 19.67 BBBB
ATOM   3423  CA  GLY B 109       4.251 -57.256 -31.023  1.00 20.03 BBBB
ATOM   3428  CA  PRO B 110       1.251 -59.478 -31.855  1.00 18.99 BBBB
ATOM   3434  CA  GLY B 111      -0.160 -56.702 -34.025  1.00 19.60 BBBB
ATOM   3438  CA  GLY B 112       3.014 -56.417 -36.074  1.00 19.97 BBBB
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ATOM   3442  CA  LEU B 113       3.265 -60.184 -36.429  1.00 19.49 BBBB
ATOM   3450  CA  ALA B 114      -0.334 -60.292 -37.661  1.00 18.70 BBBB
ATOM   3455  CA  ALA B 115       0.167 -57.516 -40.229  1.00 21.84 BBBB
ATOM   3460  CA  TRP B 116       3.365 -59.126 -41.478  1.00 23.22 BBBB
ATOM   3474  CA  SER B 117       1.735 -62.573 -41.873  1.00 22.61 BBBB
ATOM   3480  CA  LEU B 118      -1.069 -60.957 -43.882  1.00 25.70 BBBB
ATOM   3488  CA  GLY B 119       1.354 -59.174 -46.192  1.00 27.80 BBBB
ATOM   3492  CA  ILE B 120       0.568 -55.744 -44.731  1.00 24.85 BBBB
ATOM   3501  CA  PRO B 121       3.625 -53.477 -44.591  1.00 22.63 BBBB
ATOM   3507  CA  VAL B 122       4.743 -52.594 -41.083  1.00 22.03 BBBB
ATOM   3514  CA  VAL B 123       6.200 -49.184 -40.310  1.00 20.82 BBBB
ATOM   3521  CA  LEU B 124       7.749 -48.485 -36.915  1.00 22.10 BBBB
ATOM   3528  N   HIS B 125       8.182 -46.638 -35.447  1.00 21.40 BBBB
ATOM   3529  CA  HIS B 125       8.814 -45.413 -34.981  1.00 21.42 BBBB
ATOM   3530  CB  HIS B 125       7.858 -44.218 -35.067  1.00 21.57 BBBB
ATOM   3531  CG  HIS B 125       8.432 -42.948 -34.511  1.00 23.73 BBBB
ATOM   3532  CD2 HIS B 125       8.300 -42.368 -33.295  1.00 22.15 BBBB
ATOM   3533  ND1 HIS B 125       9.274 -42.127 -35.236  1.00 26.23 BBBB
ATOM   3534  CE1 HIS B 125       9.631 -41.095 -34.490  1.00 24.20 BBBB
ATOM   3535  NE2 HIS B 125       9.054 -41.218 -33.307  1.00 26.07 BBBB
ATOM   3536  C   HIS B 125       9.196 -45.642 -33.519  1.00 21.70 BBBB
ATOM   3537  O   HIS B 125       8.378 -46.117 -32.725  1.00 19.81 BBBB
ATOM   3538  N   GLU B 126      10.444 -45.332 -33.186  1.00 21.20 BBBB
ATOM   3539  CA  GLU B 126      10.947 -45.452 -31.817  1.00 22.15 BBBB
ATOM   3540  CB  GLU B 126      12.252 -46.246 -31.790  1.00 21.99 BBBB
ATOM   3541  CG  GLU B 126      12.958 -46.206 -30.439  1.00 22.04 BBBB
ATOM   3542  CD  GLU B 126      12.119 -46.824 -29.338  1.00 21.43 BBBB
ATOM   3543  OE1 GLU B 126      11.767 -48.014 -29.471  1.00 21.92 BBBB
ATOM   3544  OE2 GLU B 126      11.807 -46.124 -28.349  1.00 21.08 BBBB
ATOM   3545  C   GLU B 126      11.205 -44.027 -31.326  1.00 21.93 BBBB
ATOM   3546  O   GLU B 126      12.016 -43.300 -31.908  1.00 21.33 BBBB
ATOM   3548  CA  GLN B 127      10.682 -42.270 -29.735  1.00 22.81 BBBB
ATOM   3557  CA  ASN B 128      13.406 -43.097 -27.216  1.00 22.96 BBBB
ATOM   3565  CA  GLY B 129      17.203 -43.019 -27.294  1.00 25.36 BBBB
ATOM   3569  CA  ILE B 130      17.160 -46.716 -26.488  1.00 28.00 BBBB
ATOM   3577  CA  ALA B 131      14.978 -49.139 -28.461  1.00 25.88 BBBB
ATOM   3582  CA  GLY B 132      12.007 -50.532 -26.568  1.00 24.05 BBBB
ATOM   3586  CA  LEU B 133      11.903 -54.293 -26.020  1.00 24.54 BBBB
ATOM   3594  CA  THR B 134       9.202 -54.860 -28.639  1.00 21.22 BBBB
ATOM   3601  CA  ASN B 135      10.407 -52.419 -31.324  1.00 20.50 BBBB
ATOM   3609  CA  LYS B 136      13.886 -53.949 -31.144  1.00 22.79 BBBB
ATOM   3618  CA  TRP B 137      12.753 -57.345 -32.424  1.00 22.06 BBBB
ATOM   3632  CA  LEU B 138       9.744 -56.188 -34.431  1.00 23.15 BBBB
ATOM   3640  CA  ALA B 139      12.128 -54.092 -36.542  1.00 25.29 BBBB
ATOM   3645  CA  LYS B 140      13.279 -57.337 -38.182  1.00 28.05 BBBB
ATOM   3654  CA  ILE B 141       9.963 -57.818 -40.016  1.00 26.09 BBBB
ATOM   3662  CA  ALA B 142       9.331 -54.107 -40.498  1.00 25.03 BBBB
ATOM   3667  CA  THR B 143       9.262 -52.595 -43.984  1.00 26.10 BBBB
ATOM   3674  CA  LYS B 144      10.436 -49.238 -42.618  1.00 24.73 BBBB
ATOM   3683  CA  VAL B 145      11.947 -48.311 -39.252  1.00 23.62 BBBB
ATOM   3690  CA  MET B 146      12.338 -44.736 -37.993  1.00 23.15 BBBB
ATOM   3698  CA  GLN B 147      13.762 -43.418 -34.712  1.00 25.05 BBBB
ATOM   3707  CA  ALA B 148      13.559 -40.032 -33.009  1.00 26.88 BBBB
ATOM   3712  CA  PHE B 149      17.239 -39.820 -32.098  1.00 29.39 BBBB
ATOM   3724  CA  PRO B 150      20.310 -41.541 -33.535  1.00 31.87 BBBB
ATOM   3730  CA  GLY B 151      21.629 -44.537 -31.595  1.00 32.62 BBBB
ATOM   3734  CA  ALA B 152      18.447 -46.476 -30.753  1.00 32.71 BBBB
ATOM   3739  CA  PHE B 153      18.925 -48.506 -33.937  1.00 34.83 BBBB
ATOM   3751  CA  PRO B 154      22.158 -48.751 -35.993  1.00 38.97 BBBB
ATOM   3757  CA  ASN B 155      20.765 -47.568 -39.346  1.00 41.08 BBBB
ATOM   3765  CA  ALA B 156      17.170 -46.407 -38.843  1.00 37.55 BBBB
ATOM   3770  CA  GLU B 157      16.367 -43.044 -40.460  1.00 34.40 BBBB
ATOM   3779  CA  VAL B 158      16.337 -40.344 -37.764  1.00 31.16 BBBB
ATOM   3786  CA  VAL B 159      13.155 -38.265 -37.889  1.00 28.10 BBBB
ATOM   3793  CA  GLY B 160      12.724 -36.921 -34.355  1.00 26.93 BBBB
ATOM   3797  CA  ASN B 161       9.456 -36.807 -32.375  1.00 25.27 BBBB
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ATOM   3806  CA  PRO B 162       6.315 -34.747 -33.004  1.00 26.14 BBBB
ATOM   3812  CA  VAL B 163       6.456 -31.379 -31.216  1.00 27.75 BBBB
ATOM   3819  CA  ARG B 164       3.667 -28.953 -30.246  1.00 32.36 BBBB
ATOM   3830  CA  THR B 165       3.038 -26.307 -32.924  1.00 31.74 BBBB
ATOM   3837  CA  ASP B 166       3.252 -23.404 -30.466  1.00 30.64 BBBB
ATOM   3845  CA  VAL B 167       6.746 -24.503 -29.440  1.00 25.91 BBBB
ATOM   3852  CA  LEU B 168       7.780 -25.002 -33.075  1.00 28.46 BBBB
ATOM   3860  CA  ALA B 169       6.580 -21.455 -33.756  1.00 31.43 BBBB
ATOM   3865  CA  LEU B 170       9.002 -19.905 -31.268  1.00 29.60 BBBB
ATOM   3874  CA  PRO B 171      11.611 -17.457 -32.642  1.00 30.11 BBBB
ATOM   3880  CA  LEU B 172      15.157 -18.780 -33.062  1.00 28.33 BBBB
ATOM   3889  CA  PRO B 173      17.450 -18.550 -29.977  1.00 25.25 BBBB
ATOM   3895  CA  GLN B 174      19.526 -15.527 -31.049  1.00 25.46 BBBB
ATOM   3904  CA  GLN B 175      16.365 -13.525 -31.718  1.00 28.47 BBBB
ATOM   3913  CA  ARG B 176      14.611 -14.635 -28.525  1.00 29.01 BBBB
ATOM   3924  CA  LEU B 177      17.673 -13.970 -26.331  1.00 29.90 BBBB
ATOM   3932  CA  ALA B 178      18.766 -10.776 -28.131  1.00 30.78 BBBB
ATOM   3937  CA  GLY B 179      19.846  -7.993 -25.784  1.00 30.10 BBBB
ATOM   3941  CA  ARG B 180      18.676  -9.965 -22.787  1.00 28.97 BBBB
ATOM   3952  CA  GLU B 181      20.545  -9.027 -19.621  1.00 31.79 BBBB
ATOM   3961  CA  GLY B 182      19.871  -9.586 -15.943  1.00 27.75 BBBB
ATOM   3966  CA  PRO B 183      19.450 -12.832 -13.913  1.00 22.93 BBBB
ATOM   3972  CA  VAL B 184      19.524 -16.146 -15.729  1.00 18.01 BBBB
ATOM   3979  CA  ARG B 185      15.873 -17.216 -16.011  1.00 17.62 BBBB
ATOM   3990  CA  VAL B 186      15.508 -20.771 -14.741  1.00 16.47 BBBB
ATOM   3997  CA  LEU B 187      12.361 -22.710 -15.604  1.00 16.75 BBBB
ATOM   4005  CA  VAL B 188      11.774 -25.775 -13.381  1.00 18.41 BBBB
ATOM   4012  CA  VAL B 189       9.298 -28.234 -14.948  1.00 22.11 BBBB
ATOM   4018  N   GLY B 190       8.111 -29.887 -13.615  1.00 25.60 BBBB
ATOM   4019  CA  GLY B 190       7.914 -31.188 -12.994  1.00 27.28 BBBB
ATOM   4020  C   GLY B 190       6.808 -32.026 -13.604  1.00 29.67 BBBB
ATOM   4021  O   GLY B 190       6.668 -33.208 -13.283  1.00 29.86 BBBB
ATOM   4022  N   GLY B 191       6.025 -31.430 -14.497  1.00 30.56 BBBB
ATOM   4023  CA  GLY B 191       4.935 -32.163 -15.115  1.00 31.94 BBBB
ATOM   4024  C   GLY B 191       3.676 -32.104 -14.269  1.00 33.11 BBBB
ATOM   4025  O   GLY B 191       3.691 -31.556 -13.165  1.00 32.14 BBBB
ATOM   4026  N   SER B 192       2.587 -32.673 -14.779  1.00 34.23 BBBB
ATOM   4027  CA  SER B 192       1.313 -32.665 -14.064  1.00 35.91 BBBB
ATOM   4028  CB  SER B 192       0.283 -33.532 -14.801  1.00 36.87 BBBB
ATOM   4029  OG  SER B 192       0.702 -34.887 -14.877  1.00 39.58 BBBB
ATOM   4030  C   SER B 192       1.419 -33.128 -12.609  1.00 36.41 BBBB
ATOM   4031  O   SER B 192       0.862 -32.499 -11.714  1.00 35.78 BBBB
ATOM   4033  CA  GLN B 193       2.292 -34.763 -11.033  1.00 38.53 BBBB
ATOM   4041  N   GLY B 194       4.291 -33.398 -10.986  1.00 36.47 BBBB
ATOM   4042  CA  GLY B 194       5.398 -32.711 -10.350  1.00 35.02 BBBB
ATOM   4043  C   GLY B 194       6.584 -33.630 -10.146  1.00 34.51 BBBB
ATOM   4044  O   GLY B 194       6.442 -34.851 -10.191  1.00 34.26 BBBB
ATOM   4045  N   ALA B 195       7.761 -33.045  -9.938  1.00 33.54 BBBB
ATOM   4046  CA  ALA B 195       8.977 -33.819  -9.709  1.00 33.12 BBBB
ATOM   4047  CB  ALA B 195      10.073 -33.387 -10.679  1.00 33.17 BBBB
ATOM   4048  C   ALA B 195       9.423 -33.590  -8.267  1.00 32.87 BBBB
ATOM   4049  O   ALA B 195       9.955 -32.533  -7.923  1.00 31.47 BBBB
ATOM   4051  CA  ARG B 196       9.538 -34.512  -6.010  1.00 32.63 BBBB
ATOM   4062  CA  ILE B 197      13.329 -34.168  -6.164  1.00 28.10 BBBB
ATOM   4070  CA  LEU B 198      13.069 -30.833  -8.003  1.00 26.58 BBBB
ATOM   4078  CA  ASN B 199      10.497 -29.447  -5.563  1.00 27.07 BBBB
ATOM   4086  CA  GLN B 200      12.955 -30.326  -2.794  1.00 30.10 BBBB
ATOM   4095  CA  THR B 201      16.215 -29.345  -4.474  1.00 27.34 BBBB
ATOM   4102  CA  MET B 202      15.567 -26.048  -6.268  1.00 23.68 BBBB
ATOM   4111  CA  PRO B 203      14.608 -23.963  -3.220  1.00 23.84 BBBB
ATOM   4117  CA  GLN B 204      18.033 -24.708  -1.684  1.00 26.34 BBBB
ATOM   4126  CA  VAL B 205      19.672 -24.033  -5.043  1.00 24.44 BBBB
ATOM   4133  CA  ALA B 206      17.980 -20.610  -5.013  1.00 22.84 BBBB
ATOM   4138  CA  ALA B 207      19.442 -19.857  -1.576  1.00 26.65 BBBB
ATOM   4143  CA  LYS B 208      22.915 -20.595  -2.919  1.00 28.31 BBBB
ATOM   4152  CA  LEU B 209      22.577 -18.640  -6.171  1.00 25.68 BBBB
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ATOM   4160  CA  GLY B 210      20.675 -15.628  -4.804  1.00 26.56 BBBB
ATOM   4164  CA  ASP B 211      20.370 -12.647  -7.190  1.00 28.28 BBBB
ATOM   4172  CA  SER B 212      22.098 -14.474 -10.067  1.00 25.73 BBBB
ATOM   4178  CA  VAL B 213      18.925 -16.308 -11.116  1.00 20.76 BBBB
ATOM   4185  CA  THR B 214      15.204 -15.726 -11.337  1.00 19.60 BBBB
ATOM   4192  CA  ILE B 215      13.076 -18.850 -11.169  1.00 18.75 BBBB
ATOM   4200  CA  TRP B 216       9.661 -19.973 -12.378  1.00 19.34 BBBB
ATOM   4214  CA  HIS B 217       9.015 -23.303 -10.680  1.00 21.06 BBBB
ATOM   4224  CA  GLN B 218       6.149 -25.594 -11.735  1.00 24.30 BBBB
ATOM   4233  CA  SER B 219       5.463 -27.800  -8.684  1.00 26.73 BBBB
ATOM   4239  CA  GLY B 220       2.855 -30.242  -9.961  1.00 30.53 BBBB
ATOM   4243  CA  LYS B 221      -0.657 -30.914  -8.628  1.00 35.12 BBBB
ATOM   4252  CA  GLY B 222      -1.195 -29.899  -5.011  1.00 35.34 BBBB
ATOM   4256  CA  SER B 223       2.451 -28.934  -4.418  1.00 33.98 BBBB
ATOM   4262  CA  GLN B 224       2.187 -25.208  -5.186  1.00 33.71 BBBB
ATOM   4271  CA  GLN B 225       1.823 -24.239  -1.519  1.00 32.32 BBBB
ATOM   4280  CA  SER B 226       4.701 -26.309  -0.122  1.00 28.30 BBBB
ATOM   4286  CA  VAL B 227       7.214 -25.247  -2.791  1.00 24.28 BBBB
ATOM   4293  CA  GLU B 228       6.178 -21.592  -2.387  1.00 27.23 BBBB
ATOM   4302  CA  GLN B 229       6.853 -22.046   1.329  1.00 28.38 BBBB
ATOM   4311  CA  ALA B 230      10.185 -23.754   0.682  1.00 26.18 BBBB
ATOM   4316  CA  TYR B 231      11.371 -20.766  -1.366  1.00 25.47 BBBB
ATOM   4328  CA  ALA B 232      10.342 -18.322   1.368  1.00 27.51 BBBB
ATOM   4333  CA  GLU B 233      12.145 -20.441   3.966  1.00 30.87 BBBB
ATOM   4342  CA  ALA B 234      15.215 -20.417   1.714  1.00 28.48 BBBB
ATOM   4347  CA  GLY B 235      15.033 -16.627   1.815  1.00 26.23 BBBB
ATOM   4351  CA  GLN B 236      14.121 -16.198  -1.870  1.00 25.53 BBBB
ATOM   4361  CA  PRO B 237      10.336 -15.587  -1.720  1.00 24.65 BBBB
ATOM   4367  CA  GLN B 238      10.277 -13.558  -4.945  1.00 24.29 BBBB
ATOM   4376  CA  HIS B 239      10.526 -16.608  -7.201  1.00 22.08 BBBB
ATOM   4386  CA  LYS B 240       7.375 -17.589  -9.105  1.00 23.26 BBBB
ATOM   4395  CA  VAL B 241       5.740 -20.911  -8.277  1.00 23.78 BBBB
ATOM   4402  CA  THR B 242       2.758 -22.301 -10.177  1.00 25.93 BBBB
ATOM   4409  CA  GLU B 243       0.999 -25.651  -9.837  1.00 27.03 BBBB
ATOM   4418  CA  PHE B 244       0.964 -26.068 -13.620  1.00 26.54 BBBB
ATOM   4429  CA  ILE B 245       1.932 -24.242 -16.802  1.00 28.48 BBBB
ATOM   4437  CA  ASP B 246      -0.754 -24.396 -19.457  1.00 36.00 BBBB
ATOM   4445  CA  ASP B 247       1.245 -22.392 -21.999  1.00 30.74 BBBB
ATOM   4453  CA  MET B 248       4.625 -24.136 -22.138  1.00 28.41 BBBB
ATOM   4461  CA  ALA B 249       5.512 -22.216 -25.290  1.00 24.67 BBBB
ATOM   4466  CA  ALA B 250       5.188 -18.933 -23.390  1.00 21.78 BBBB
ATOM   4471  CA  ALA B 251       7.301 -20.259 -20.501  1.00 20.85 BBBB
ATOM   4476  CA  TYR B 252       9.972 -21.616 -22.886  1.00 22.78 BBBB
ATOM   4488  CA  ALA B 253      10.131 -18.224 -24.636  1.00 23.54 BBBB
ATOM   4493  CA  TRP B 254      10.829 -16.534 -21.303  1.00 19.76 BBBB
ATOM   4507  CA  ALA B 255      13.399 -19.025 -20.003  1.00 19.51 BBBB
ATOM   4512  CA  ASP B 256      17.176 -19.026 -20.434  1.00 17.58 BBBB
ATOM   4520  CA  VAL B 257      17.535 -22.603 -19.194  1.00 18.53 BBBB
ATOM   4527  CA  VAL B 258      15.208 -25.456 -18.234  1.00 19.32 BBBB
ATOM   4534  CA  VAL B 259      15.581 -27.957 -15.374  1.00 19.85 BBBB
ATOM   4541  CA  CYS B 260      13.454 -31.055 -15.946  1.00 22.00 BBBB
ATOM   4546  N   ARG B 261      12.937 -33.397 -16.212  1.00 22.34 BBBB
ATOM   4547  CA  ARG B 261      13.170 -34.800 -16.515  1.00 23.75 BBBB
ATOM   4548  CB  ARG B 261      11.964 -35.663 -16.104  1.00 27.16 BBBB
ATOM   4549  CG  ARG B 261      11.376 -35.337 -14.738  1.00 31.82 BBBB
ATOM   4550  CD  ARG B 261      11.490 -36.473 -13.732  1.00 36.33 BBBB
ATOM   4551  NE  ARG B 261      12.865 -36.721 -13.323  1.00 38.48 BBBB
ATOM   4552  CZ  ARG B 261      13.218 -37.176 -12.125  1.00 37.25 BBBB
ATOM   4553  NH1 ARG B 261      12.295 -37.433 -11.204  1.00 38.46 BBBB
ATOM   4554  NH2 ARG B 261      14.499 -37.370 -11.848  1.00 36.79 BBBB
ATOM   4555  C   ARG B 261      13.351 -34.871 -18.032  1.00 23.98 BBBB
ATOM   4556  O   ARG B 261      13.117 -33.883 -18.746  1.00 22.44 BBBB
ATOM   4558  CA  SER B 262      13.975 -36.189 -19.948  1.00 23.18 BBBB
ATOM   4563  N   GLY B 263      11.850 -37.151 -20.619  1.00 22.74 BBBB
ATOM   4564  CA  GLY B 263      11.026 -38.079 -21.361  1.00 22.85 BBBB
ATOM   4565  C   GLY B 263      11.392 -37.793 -22.813  1.00 24.06 BBBB
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ATOM   4566  O   GLY B 263      11.908 -36.705 -23.121  1.00 22.75 BBBB
ATOM   4567  N   ALA B 264      11.130 -38.739 -23.708  1.00 23.37 BBBB
ATOM   4568  CA  ALA B 264      11.482 -38.564 -25.115  1.00 24.25 BBBB
ATOM   4569  CB  ALA B 264      11.133 -39.829 -25.894  1.00 24.58 BBBB
ATOM   4570  C   ALA B 264      10.843 -37.343 -25.783  1.00 24.29 BBBB
ATOM   4571  O   ALA B 264      11.523 -36.572 -26.470  1.00 24.33 BBBB
ATOM   4573  CA  LEU B 265       8.846 -36.037 -26.205  1.00 24.66 BBBB
ATOM   4581  CA  THR B 266      10.194 -33.557 -23.657  1.00 22.34 BBBB
ATOM   4588  CA  VAL B 267      13.730 -33.762 -25.023  1.00 21.11 BBBB
ATOM   4595  CA  SER B 268      12.411 -33.191 -28.567  1.00 21.96 BBBB
ATOM   4600  N   GLU B 269      10.928 -31.563 -27.557  1.00 21.64 BBBB
ATOM   4601  CA  GLU B 269      10.282 -30.272 -27.378  1.00 21.95 BBBB
ATOM   4602  CB  GLU B 269       9.213 -30.399 -26.292  1.00 24.72 BBBB
ATOM   4603  CG  GLU B 269       8.480 -29.128 -25.940  1.00 27.67 BBBB
ATOM   4604  CD  GLU B 269       7.385 -29.380 -24.908  1.00 30.05 BBBB
ATOM   4605  OE1 GLU B 269       6.325 -29.915 -25.287  1.00 31.50 BBBB
ATOM   4606  OE2 GLU B 269       7.591 -29.057 -23.719  1.00 29.84 BBBB
ATOM   4607  C   GLU B 269      11.321 -29.214 -26.999  1.00 21.68 BBBB
ATOM   4608  O   GLU B 269      11.301 -28.095 -27.518  1.00 18.12 BBBB
ATOM   4610  CA  ILE B 270      13.295 -28.698 -25.638  1.00 20.62 BBBB
ATOM   4618  CA  ALA B 271      15.440 -29.058 -28.776  1.00 22.45 BBBB
ATOM   4623  CA  ALA B 272      12.719 -27.451 -30.898  1.00 22.17 BBBB
ATOM   4628  CA  ALA B 273      12.361 -24.596 -28.407  1.00 21.97 BBBB
ATOM   4633  CA  GLY B 274      16.093 -24.023 -28.709  1.00 21.07 BBBB
ATOM   4637  CA  LEU B 275      16.666 -24.057 -24.966  1.00 19.78 BBBB
ATOM   4646  CA  PRO B 276      19.651 -25.199 -22.875  1.00 16.62 BBBB
ATOM   4652  CA  ALA B 277      18.638 -27.807 -20.321  1.00 15.80 BBBB
ATOM   4657  CA  LEU B 278      19.896 -29.429 -17.145  1.00 18.48 BBBB
ATOM   4665  CA  PHE B 279      18.266 -32.838 -17.392  1.00 21.59 BBBB
ATOM   4676  CA  VAL B 280      17.502 -34.902 -14.281  1.00 25.67 BBBB
ATOM   4682  N   PRO B 281      17.324 -37.080 -15.370  1.00 27.08 BBBB
ATOM   4683  CD  PRO B 281      18.750 -37.057 -15.726  1.00 27.31 BBBB
ATOM   4684  CA  PRO B 281      16.698 -38.320 -15.824  1.00 29.05 BBBB
ATOM   4685  CB  PRO B 281      17.851 -39.071 -16.492  1.00 29.44 BBBB
ATOM   4686  CG  PRO B 281      18.791 -37.992 -16.895  1.00 29.67 BBBB
ATOM   4687  C   PRO B 281      16.092 -39.121 -14.684  1.00 31.51 BBBB
ATOM   4688  O   PRO B 281      16.675 -39.223 -13.603  1.00 32.26 BBBB
ATOM   4690  CA  PHE B 282      14.246 -40.496 -13.926  1.00 37.13 BBBB
ATOM   4701  CA  GLN B 283      16.319 -43.395 -12.591  1.00 41.11 BBBB
ATOM   4710  CA  HIS B 284      15.641 -46.917 -13.843  1.00 43.69 BBBB
ATOM   4720  CA  LYS B 285      17.767 -49.993 -14.571  1.00 45.34 BBBB
ATOM   4729  CA  ASP B 286      16.949 -49.299 -18.222  1.00 43.26 BBBB
ATOM   4737  CA  ARG B 287      17.951 -45.623 -17.883  1.00 36.28 BBBB
ATOM   4748  CA  GLN B 288      15.622 -44.804 -20.755  1.00 30.77 BBBB
ATOM   4756  N   GLN B 289      15.378 -42.554 -19.857  1.00 29.38 BBBB
ATOM   4757  CA  GLN B 289      15.474 -41.099 -19.904  1.00 29.46 BBBB
ATOM   4758  CB  GLN B 289      14.772 -40.472 -18.700  1.00 29.25 BBBB
ATOM   4759  CG  GLN B 289      13.265 -40.416 -18.883  1.00 29.32 BBBB
ATOM   4760  CD  GLN B 289      12.575 -39.585 -17.826  1.00 29.84 BBBB
ATOM   4761  OE1 GLN B 289      13.191 -38.728 -17.188  1.00 29.52 BBBB
ATOM   4762  NE2 GLN B 289      11.281 -39.821 -17.647  1.00 28.95 BBBB
ATOM   4763  C   GLN B 289      16.906 -40.613 -20.005  1.00 29.36 BBBB
ATOM   4764  O   GLN B 289      17.173 -39.557 -20.585  1.00 29.12 BBBB
ATOM   4766  CA  TYR B 290      19.228 -40.984 -19.550  1.00 29.55 BBBB
ATOM   4778  CA  TRP B 291      19.542 -42.282 -23.116  1.00 28.07 BBBB
ATOM   4791  N   ASN B 292      17.658 -40.779 -23.508  1.00 25.52 BBBB
ATOM   4792  CA  ASN B 292      16.902 -39.784 -24.270  1.00 26.06 BBBB
ATOM   4793  CB  ASN B 292      15.484 -39.599 -23.709  1.00 24.78 BBBB
ATOM   4794  CG  ASN B 292      14.590 -40.811 -23.928  1.00 24.46 BBBB
ATOM   4795  OD1 ASN B 292      14.842 -41.641 -24.798  1.00 25.33 BBBB
ATOM   4796  ND2 ASN B 292      13.523 -40.900 -23.146  1.00 23.83 BBBB
ATOM   4797  C   ASN B 292      17.605 -38.427 -24.258  1.00 25.99 BBBB
ATOM   4798  O   ASN B 292      17.566 -37.687 -25.244  1.00 26.18 BBBB
ATOM   4799  N   ALA B 293      18.242 -38.105 -23.139  1.00 25.66 BBBB
ATOM   4800  CA  ALA B 293      18.926 -36.822 -22.979  1.00 25.69 BBBB
ATOM   4801  CB  ALA B 293      18.940 -36.422 -21.506  1.00 24.17 BBBB
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ATOM   4802  C   ALA B 293      20.346 -36.800 -23.521  1.00 25.67 BBBB
ATOM   4803  O   ALA B 293      20.855 -35.743 -23.902  1.00 25.52 BBBB
ATOM   4805  CA  LEU B 294      22.354 -38.088 -24.032  1.00 25.90 BBBB
ATOM   4814  CA  PRO B 295      21.998 -36.870 -27.635  1.00 26.15 BBBB
ATOM   4820  CA  LEU B 296      21.521 -33.265 -26.481  1.00 25.42 BBBB
ATOM   4828  CA  GLU B 297      24.354 -33.530 -23.953  1.00 28.78 BBBB
ATOM   4837  CA  LYS B 298      26.644 -34.947 -26.648  1.00 31.90 BBBB
ATOM   4846  CA  ALA B 299      25.773 -31.965 -28.847  1.00 30.38 BBBB
ATOM   4851  CA  GLY B 300      26.777 -29.635 -26.017  1.00 26.18 BBBB
ATOM   4855  CA  ALA B 301      23.214 -28.333 -25.638  1.00 22.50 BBBB
ATOM   4860  CA  ALA B 302      22.516 -29.770 -22.186  1.00 21.78 BBBB
ATOM   4865  CA  LYS B 303      23.979 -31.340 -19.048  1.00 25.86 BBBB
ATOM   4874  CA  ILE B 304      22.753 -34.598 -17.550  1.00 27.17 BBBB
ATOM   4882  CA  ILE B 305      22.843 -35.178 -13.813  1.00 29.01 BBBB
ATOM   4890  CA  GLU B 306      21.664 -38.702 -13.061  1.00 34.65 BBBB
ATOM   4899  CA  GLN B 307      20.377 -39.599  -9.613  1.00 40.54 BBBB
ATOM   4909  CA  PRO B 308      23.828 -40.891  -8.484  1.00 43.20 BBBB
ATOM   4915  CA  GLN B 309      25.247 -37.361  -8.787  1.00 43.46 BBBB
ATOM   4924  CA  LEU B 310      22.232 -35.166  -8.022  1.00 39.65 BBBB
ATOM   4932  CA  SER B 311      22.660 -32.714  -5.154  1.00 34.90 BBBB
ATOM   4938  CA  VAL B 312      21.990 -29.074  -4.341  1.00 31.50 BBBB
ATOM   4945  CA  ASP B 313      25.642 -28.202  -4.957  1.00 29.61 BBBB
ATOM   4953  CA  ALA B 314      25.782 -30.099  -8.254  1.00 26.47 BBBB
ATOM   4958  CA  VAL B 315      22.755 -28.215  -9.612  1.00 25.33 BBBB
ATOM   4965  CA  ALA B 316      23.888 -24.872  -8.199  1.00 27.13 BBBB
ATOM   4970  CA  ASN B 317      27.444 -25.246  -9.518  1.00 28.52 BBBB
ATOM   4978  CA  THR B 318      26.174 -26.371 -12.906  1.00 27.04 BBBB
ATOM   4985  CA  LEU B 319      23.883 -23.370 -13.357  1.00 25.21 BBBB
ATOM   4993  CA  ALA B 320      26.445 -20.931 -11.957  1.00 24.59 BBBB
ATOM   4998  CA  GLY B 321      28.934 -22.031 -14.591  1.00 24.34 BBBB
ATOM   5002  CA  TRP B 322      26.738 -21.007 -17.521  1.00 21.72 BBBB
ATOM   5016  CA  SER B 323      27.141 -17.404 -18.692  1.00 19.04 BBBB
ATOM   5022  CA  ARG B 324      24.725 -15.741 -21.112  1.00 18.09 BBBB
ATOM   5033  CA  GLU B 325      27.220 -16.368 -23.954  1.00 16.96 BBBB
ATOM   5042  CA  THR B 326      27.460 -20.055 -23.070  1.00 16.39 BBBB
ATOM   5049  CA  LEU B 327      23.659 -20.305 -22.780  1.00 17.27 BBBB
ATOM   5057  CA  LEU B 328      23.175 -18.745 -26.222  1.00 17.39 BBBB
ATOM   5065  CA  THR B 329      25.567 -21.335 -27.688  1.00 21.30 BBBB
ATOM   5072  CA  MET B 330      23.771 -24.153 -25.870  1.00 19.91 BBBB
ATOM   5080  CA  ALA B 331      20.412 -22.871 -27.098  1.00 18.49 BBBB
ATOM   5085  CA  GLU B 332      21.626 -22.827 -30.704  1.00 21.47 BBBB
ATOM   5094  CA  ARG B 333      23.040 -26.330 -30.408  1.00 23.77 BBBB
ATOM   5105  CA  ALA B 334      19.648 -27.420 -29.063  1.00 22.88 BBBB
ATOM   5110  CA  ARG B 335      17.795 -25.892 -32.002  1.00 23.54 BBBB
ATOM   5121  CA  ALA B 336      20.330 -27.477 -34.372  1.00 26.85 BBBB
ATOM   5126  CA  ALA B 337      19.740 -30.925 -32.865  1.00 30.89 BBBB
ATOM   5131  CA  SER B 338      16.008 -30.432 -33.408  1.00 32.41 BBBB
ATOM   5137  CA  ILE B 339      13.882 -31.941 -36.187  1.00 34.35 BBBB
ATOM   5146  CA  PRO B 340      10.733 -29.730 -36.600  1.00 34.94 BBBB
ATOM   5152  CA  ASP B 341       8.711 -31.820 -39.056  1.00 33.33 BBBB
ATOM   5160  CA  ALA B 342       8.875 -35.238 -37.411  1.00 29.09 BBBB
ATOM   5165  CA  THR B 343       5.115 -35.696 -37.744  1.00 28.55 BBBB
ATOM   5172  CA  GLU B 344       5.085 -34.933 -41.480  1.00 32.00 BBBB
ATOM   5181  CA  ARG B 345       8.138 -37.123 -42.067  1.00 31.44 BBBB
ATOM   5192  CA  VAL B 346       6.578 -40.151 -40.384  1.00 28.61 BBBB
ATOM   5199  CA  ALA B 347       3.249 -39.617 -42.137  1.00 28.96 BBBB
ATOM   5204  CA  ASN B 348       5.035 -39.286 -45.493  1.00 34.56 BBBB
ATOM   5212  CA  GLU B 349       6.954 -42.540 -44.956  1.00 34.86 BBBB
ATOM   5221  CA  VAL B 350       3.767 -44.306 -43.919  1.00 33.79 BBBB
ATOM   5228  CA  SER B 351       2.196 -42.946 -47.095  1.00 36.67 BBBB
ATOM   5234  CA  ARG B 352       5.114 -44.088 -49.251  1.00 40.03 BBBB
ATOM   5245  CA  VAL B 353       5.089 -47.587 -47.737  1.00 42.78 BBBB
ATOM   5252  CA  ALA B 354       1.336 -47.957 -48.212  1.00 47.24 BBBB
ATOM   5257  CA  ARG B 355       2.035 -46.964 -51.824  1.00 52.71 BBBB
ATOM   5268  CA  ALA B 356       4.453 -49.913 -51.809  1.00 54.93 BBBB
ATOM   5273  CA  LEU B 357       7.023 -47.522 -53.289  1.00 57.81 BBBB
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END

TABLE 4 ATOMIC COORDINATES OF THE DONOR NUCLEOTIDE BINDING SITE

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REMARK    4 1MUR COMPLIES WITH FORMAT V. 2.0, 11-MAY-2000
ATOM      1  N   LEU B 187      13.695 -22.128 -15.588  1.00 15.92      N
ATOM      2  CA  LEU B 187      12.361 -22.710 -15.604  1.00 16.75      C
ATOM      3  C   LEU B 187      12.450 -24.146 -15.085  1.00 16.85      C
ATOM      4  O   LEU B 187      13.115 -24.982 -15.688  1.00 17.18      O
ATOM      5  CB  LEU B 187      11.813 -22.701 -17.035  1.00 16.85      C
ATOM      6  CG  LEU B 187      10.445 -23.340 -17.276  1.00 18.63      C
ATOM      7  CD1 LEU B 187       9.368 -22.478 -16.625  1.00 19.42      C
ATOM      8  CD2 LEU B 187      10.198 -23.449 -18.783  1.00 19.11      C
ATOM      9  N   VAL B 188      11.788 -24.426 -13.964  1.00 18.20      N
ATOM     10  CA  VAL B 188      11.774 -25.775 -13.381  1.00 18.41      C
ATOM     11  C   VAL B 188      10.434 -26.440 -13.739  1.00 19.88      C
ATOM     12  O   VAL B 188       9.371 -25.967 -13.336  1.00 20.39      O
ATOM     13  CB  VAL B 188      11.902 -25.714 -11.842  1.00 18.98      C
ATOM     14  CG1 VAL B 188      12.088 -27.126 -11.270  1.00 18.50      C
ATOM     15  CG2 VAL B 188      13.061 -24.818 -11.449  1.00 18.83      C
ATOM     16  N   VAL B 189      10.493 -27.532 -14.496  1.00 21.55      N
ATOM     17  CA  VAL B 189       9.298 -28.234 -14.948  1.00 22.11      C
ATOM     18  C   VAL B 189       9.191 -29.639 -14.351  1.00 23.90      C
ATOM     19  O   VAL B 189      10.067 -30.478 -14.559  1.00 23.61      O
ATOM     20  CB  VAL B 189       9.299 -28.342 -16.488  1.00 22.50      C
ATOM     21  CG1 VAL B 189       8.009 -29.013 -16.981  1.00 22.70      C
ATOM     22  CG2 VAL B 189       9.470 -26.943 -17.101  1.00 21.26      C
ATOM     23  N   GLY B 190       8.111 -29.887 -13.615  1.00 25.60      N
ATOM     24  CA  GLY B 190       7.914 -31.188 -12.994  1.00 27.28      C
ATOM     25  C   GLY B 190       6.808 -32.026 -13.604  1.00 29.67      C
ATOM     26  O   GLY B 190       6.668 -33.208 -13.283  1.00 29.86      O
ATOM     27  N   GLY B 191       6.025 -31.430 -14.497  1.00 30.56      N
ATOM     28  CA  GLY B 191       4.935 -32.163 -15.115  1.00 31.94      C
ATOM     29  C   GLY B 191       3.676 -32.104 -14.269  1.00 33.11      C
ATOM     30  O   GLY B 191       3.691 -31.556 -13.165  1.00 32.14      O
ATOM     31  N   ALA B 195       7.761 -33.045  -9.938  1.00 33.54      N
ATOM     32  CA  ALA B 195       8.977 -33.819  -9.709  1.00 33.12      C
ATOM     33  C   ALA B 195       9.423 -33.590  -8.267  1.00 32.87      C
ATOM     34  O   ALA B 195       9.955 -32.533  -7.923  1.00 31.47      O
ATOM     35  CB  ALA B 195      10.073 -33.387 -10.679  1.00 33.17      C
ATOM     36  N   LEU B 198      12.897 -32.223  -7.590  1.00 27.07      N
ATOM     37  CA  LEU B 198      13.069 -30.833  -8.003  1.00 26.58      C
ATOM     38  C   LEU B 198      12.388 -29.893  -7.006  1.00 26.41      C
ATOM     39  O   LEU B 198      12.930 -28.835  -6.667  1.00 26.35      O
ATOM     40  CB  LEU B 198      12.504 -30.616  -9.412  1.00 25.88      C
ATOM     41  CG  LEU B 198      13.196 -31.408 -10.524  1.00 25.40      C
ATOM     42  CD1 LEU B 198      12.625 -31.007 -11.874  1.00 26.54      C
ATOM     43  CD2 LEU B 198      14.692 -31.146 -10.493  1.00 25.94      C
ATOM     44  N   TYR B 252       8.723 -21.314 -22.184  1.00 21.27      N
ATOM     45  CA  TYR B 252       9.972 -21.616 -22.886  1.00 22.78      C
ATOM     46  C   TYR B 252      10.566 -20.354 -23.516  1.00 23.57      C
ATOM     47  O   TYR B 252      11.784 -20.180 -23.550  1.00 23.91      O
ATOM     48  CB  TYR B 252       9.726 -22.661 -23.980  1.00 21.62      C
ATOM     49  CG  TYR B 252       9.662 -24.100 -23.505  1.00 23.34      C
ATOM     50  CD1 TYR B 252       9.003 -25.065 -24.261  1.00 22.88      C
ATOM     51  CD2 TYR B 252      10.288 -24.505 -22.319  1.00 22.30      C
ATOM     52  CE1 TYR B 252       8.961 -26.392 -23.861  1.00 24.81      C
ATOM     53  CE2 TYR B 252      10.253 -25.838 -21.912  1.00 23.56      C
ATOM     54  CZ  TYR B 252       9.590 -26.772 -22.687  1.00 24.26      C
ATOM     55  OH  TYR B 252       9.554 -28.088 -22.305  1.00 25.57      O
ATOM     56  N   VAL B 258      16.263 -24.643 -18.818  1.00 18.74      N
ATOM     57  CA  VAL B 258      15.208 -25.456 -18.234  1.00 19.32      C
ATOM     58  C   VAL B 258      15.799 -26.585 -17.389  1.00 19.70      C
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ATOM     59  O   VAL B 258      16.808 -27.175 -17.758  1.00 18.96      O
ATOM     60  CB  VAL B 258      14.328 -26.100 -19.337  1.00 19.89      C
ATOM     61  CG1 VAL B 258      13.101 -26.754 -18.714  1.00 19.81      C
ATOM     62  CG2 VAL B 258      13.907 -25.041 -20.364  1.00 21.59      C
ATOM     63  N   VAL B 259      15.167 -26.861 -16.253  1.00 20.24      N
ATOM     64  CA  VAL B 259      15.581 -27.957 -15.374  1.00 19.85      C
ATOM     65  C   VAL B 259      14.382 -28.890 -15.371  1.00 20.02      C
ATOM     66  O   VAL B 259      13.301 -28.500 -14.942  1.00 21.88      O
ATOM     67  CB  VAL B 259      15.850 -27.483 -13.936  1.00 20.08      C
ATOM     68  CG1 VAL B 259      16.222 -28.689 -13.059  1.00 20.22      C
ATOM     69  CG2 VAL B 259      16.966 -26.453 -13.930  1.00 17.86      C
ATOM     70  N   CYS B 260      14.562 -30.111 -15.867  1.00 21.70      N
ATOM     71  CA  CYS B 260      13.454 -31.055 -15.946  1.00 22.00      C
ATOM     72  C   CYS B 260      13.903 -32.478 -16.242  1.00 21.86      C
ATOM     73  O   CYS B 260      15.087 -32.730 -16.496  1.00 21.34      O
ATOM     74  CB  CYS B 260      12.494 -30.618 -17.057  1.00 22.77      C
ATOM     75  SG  CYS B 260      13.297 -30.506 -18.711  1.00 22.15      S
ATOM     76  N   ARG B 261      12.937 -33.397 -16.212  1.00 22.34      N
ATOM     77  CA  ARG B 261      13.170 -34.800 -16.515  1.00 23.75      C
ATOM     78  C   ARG B 261      13.351 -34.871 -18.032  1.00 23.98      C
ATOM     79  O   ARG B 261      13.117 -33.883 -18.746  1.00 22.44      O
ATOM     80  CB  ARG B 261      11.964 -35.663 -16.104  1.00 27.16      C
ATOM     81  CG  ARG B 261      11.376 -35.337 -14.738  1.00 31.82      C
ATOM     82  CD  ARG B 261      11.490 -36.473 -13.732  1.00 36.33      C
ATOM     83  NE  ARG B 261      12.865 -36.721 -13.323  1.00 38.48      N
ATOM     84  CZ  ARG B 261      13.218 -37.176 -12.125  1.00 37.25      C
ATOM     85  NH1 ARG B 261      12.295 -37.433 -11.204  1.00 38.46      N
ATOM     86  NH2 ARG B 261      14.499 -37.370 -11.848  1.00 36.79      N
ATOM     87  N   SER B 262      13.740 -36.038 -18.527  1.00 22.00      N
ATOM     88  CA  SER B 262      13.975 -36.189 -19.948  1.00 23.18      C
ATOM     89  C   SER B 262      13.173 -37.263 -20.676  1.00 22.90      C
ATOM     90  O   SER B 262      13.738 -38.179 -21.274  1.00 23.25      O
ATOM     91  CB  SER B 262      15.481 -36.377 -20.203  1.00 24.45      C
ATOM     92  OG  SER B 262      16.043 -37.326 -19.311  1.00 25.79      O
ATOM     93  N   GLY B 263      11.850 -37.151 -20.619  1.00 22.74      N
ATOM     94  CA  GLY B 263      11.026 -38.079 -21.361  1.00 22.85      C
ATOM     95  C   GLY B 263      11.392 -37.793 -22.813  1.00 24.06      C
ATOM     96  O   GLY B 263      11.908 -36.705 -23.121  1.00 22.75      O
ATOM     97  N   ALA B 264      11.130 -38.739 -23.708  1.00 23.37      N
ATOM     98  CA  ALA B 264      11.482 -38.564 -25.115  1.00 24.25      C
ATOM     99  C   ALA B 264      10.843 -37.343 -25.783  1.00 24.29      C
ATOM    100  O   ALA B 264      11.523 -36.572 -26.470  1.00 24.33      O
ATOM    101  CB  ALA B 264      11.133 -39.829 -25.894  1.00 24.58      C
ATOM    102  N   LEU B 265       9.541 -37.167 -25.596  1.00 24.44      N
ATOM    103  CA  LEU B 265       8.846 -36.037 -26.205  1.00 24.66      C
ATOM    104  C   LEU B 265       9.331 -34.717 -25.613  1.00 24.47      C
ATOM    105  O   LEU B 265       9.374 -33.693 -26.301  1.00 23.85      O
ATOM    106  CB  LEU B 265       7.332 -36.183 -26.011  1.00 25.33      C
ATOM    107  CG  LEU B 265       6.760 -37.544 -26.426  1.00 27.97      C
ATOM    108  CD1 LEU B 265       5.242 -37.541 -26.258  1.00 28.21      C
ATOM    109  CD2 LEU B 265       7.146 -37.856 -27.878  1.00 27.40      C
ATOM    110  N   THR B 266       9.702 -34.747 -24.338  1.00 22.12      N
ATOM    111  CA  THR B 266      10.194 -33.557 -23.657  1.00 22.34      C
ATOM    112  C   THR B 266      11.535 -33.117 -24.226  1.00 21.15      C
ATOM    113  O   THR B 266      11.761 -31.926 -24.442  1.00 20.35      O
ATOM    114  CB  THR B 266      10.348 -33.803 -22.140  1.00 22.35      C
ATOM    115  OG1 THR B 266       9.061 -34.087 -21.583  1.00 24.46      O
ATOM    116  CG2 THR B 266      10.945 -32.573 -21.444  1.00 24.00      C
ATOM    117  N   VAL B 267      12.427 -34.075 -24.461  1.00 20.46      N
ATOM    118  CA  VAL B 267      13.730 -33.762 -25.023  1.00 21.11      C
ATOM    119  C   VAL B 267      13.548 -33.138 -26.416  1.00 21.34      C
ATOM    120  O   VAL B 267      14.188 -32.135 -26.747  1.00 19.99      O
ATOM    121  CB  VAL B 267      14.614 -35.039 -25.114  1.00 21.54      C
ATOM    122  CG1 VAL B 267      15.903 -34.740 -25.865  1.00 20.72      C
ATOM    123  CG2 VAL B 267      14.938 -35.541 -23.708  1.00 20.45      C
ATOM    124  N   SER B 268      12.663 -33.717 -27.222  1.00 21.61      N
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ATOM    125  CA  SER B 268      12.411 -33.191 -28.567  1.00 21.96      C
ATOM    126  C   SER B 268      11.817 -31.790 -28.519  1.00 21.81      C
ATOM    127  O   SER B 268      12.158 -30.933 -29.336  1.00 22.60      O
ATOM    128  CB  SER B 268      11.474 -34.121 -29.344  1.00 21.57      C
ATOM    129  OG  SER B 268      12.141 -35.316 -29.721  1.00 24.06      O
ATOM    130  N   GLU B 269      10.928 -31.563 -27.557  1.00 21.64      N
ATOM    131  CA  GLU B 269      10.282 -30.272 -27.378  1.00 21.95      C
ATOM    132  C   GLU B 269      11.321 -29.214 -26.999  1.00 21.68      C
ATOM    133  O   GLU B 269      11.301 -28.095 -27.518  1.00 18.12      O
ATOM    134  CB  GLU B 269       9.213 -30.399 -26.292  1.00 24.72      C
ATOM    135  CG  GLU B 269       8.480 -29.128 -25.940  1.00 27.67      C
ATOM    136  CD  GLU B 269       7.385 -29.380 -24.908  1.00 30.05      C
ATOM    137  OE1 GLU B 269       6.325 -29.915 -25.287  1.00 31.50      O
ATOM    138  OE2 GLU B 269       7.591 -29.057 -23.719  1.00 29.84      O
ATOM    139  N   ILE B 270      12.224 -29.581 -26.092  1.00 19.43      N
ATOM    140  CA  ILE B 270      13.295 -28.698 -25.638  1.00 20.62      C
ATOM    141  C   ILE B 270      14.214 -28.314 -26.806  1.00 20.58      C
ATOM    142  O   ILE B 270      14.595 -27.151 -26.954  1.00 20.50      O
ATOM    143  CB  ILE B 270      14.157 -29.391 -24.533  1.00 20.30      C
ATOM    144  CG1 ILE B 270      13.337 -29.574 -23.254  1.00 21.32      C
ATOM    145  CG2 ILE B 270      15.415 -28.595 -24.266  1.00 19.17      C
ATOM    146  CD1 ILE B 270      12.926 -28.291 -22.583  1.00 23.40      C
ATOM    147  N   ALA B 277      19.316 -27.110 -21.396  1.00 17.01      N
ATOM    148  CA  ALA B 277      18.638 -27.807 -20.321  1.00 15.80      C
ATOM    149  C   ALA B 277      19.591 -28.526 -19.382  1.00 17.37      C
ATOM    150  O   ALA B 277      20.710 -28.891 -19.755  1.00 17.09      O
ATOM    151  CB  ALA B 277      17.641 -28.805 -20.895  1.00 17.01      C
ATOM    152  N   LEU B 278      19.147 -28.673 -18.138  1.00 17.14      N
ATOM    153  CA  LEU B 278      19.896 -29.429 -17.145  1.00 18.48      C
ATOM    154  C   LEU B 278      18.884 -30.535 -16.898  1.00 19.62      C
ATOM    155  O   LEU B 278      17.870 -30.330 -16.218  1.00 20.77      O
ATOM    156  CB  LEU B 278      20.140 -28.619 -15.869  1.00 19.19      C
ATOM    157  CG  LEU B 278      21.084 -29.308 -14.868  1.00 20.85      C
ATOM    158  CD1 LEU B 278      21.283 -28.411 -13.668  1.00 21.11      C
ATOM    159  CD2 LEU B 278      20.497 -30.647 -14.433  1.00 19.16      C
ATOM    160  N   PHE B 279      19.149 -31.691 -17.495  1.00 19.50      N
ATOM    161  CA  PHE B 279      18.266 -32.838 -17.392  1.00 21.59      C
ATOM    162  C   PHE B 279      18.525 -33.709 -16.167  1.00 22.86      C
ATOM    163  O   PHE B 279      19.671 -34.065 -15.871  1.00 23.32      O
ATOM    164  CB  PHE B 279      18.385 -33.700 -18.651  1.00 21.07      C
ATOM    165  CG  PHE B 279      17.740 -33.099 -19.876  1.00 19.35      C
ATOM    166  CD1 PHE B 279      18.481 -32.898 -21.035  1.00 19.42      C
ATOM    167  CD2 PHE B 279      16.379 -32.794 -19.888  1.00 18.16      C
ATOM    168  CE1 PHE B 279      17.874 -32.405 -22.203  1.00 19.06      C
ATOM    169  CE2 PHE B 279      15.759 -32.298 -21.052  1.00 17.65      C
ATOM    170  CZ  PHE B 279      16.515 -32.108 -22.208  1.00 15.61      C
ATOM    171  N   VAL B 280      17.445 -34.037 -15.461  1.00 23.88      N
ATOM    172  CA  VAL B 280      17.502 -34.902 -14.281  1.00 25.67      C
ATOM    173  C   VAL B 280      16.690 -36.136 -14.658  1.00 25.65      C
ATOM    174  O   VAL B 280      15.509 -36.239 -14.346  1.00 24.57      O
ATOM    175  CB  VAL B 280      16.883 -34.223 -13.048  1.00 26.89      C
ATOM    176  CG1 VAL B 280      16.954 -35.159 -11.847  1.00 28.12      C
ATOM    177  CG2 VAL B 280      17.631 -32.929 -12.742  1.00 27.70      C
ATOM    178  N   PRO B 281      17.324 -37.080 -15.370  1.00 27.08      N
ATOM    179  CA  PRO B 281      16.698 -38.320 -15.824  1.00 29.05      C
ATOM    180  C   PRO B 281      16.092 -39.121 -14.684  1.00 31.51      C
ATOM    181  O   PRO B 281      16.675 -39.223 -13.603  1.00 32.26      O
ATOM    182  CB  PRO B 281      17.851 -39.071 -16.492  1.00 29.44      C
ATOM    183  CG  PRO B 281      18.791 -37.992 -16.895  1.00 29.67      C
ATOM    184  CD  PRO B 281      18.750 -37.057 -15.726  1.00 27.31      C
ATOM    185  N   PHE B 282      14.908 -39.668 -14.923  1.00 33.83      N
ATOM    186  CA  PHE B 282      14.246 -40.496 -13.926  1.00 37.13      C
ATOM    187  C   PHE B 282      15.078 -41.776 -13.880  1.00 38.09      C
ATOM    188  O   PHE B 282      15.357 -42.373 -14.921  1.00 38.33      O
ATOM    189  CB  PHE B 282      12.818 -40.808 -14.372  1.00 38.38      C
ATOM    190  CG  PHE B 282      12.032 -41.606 -13.377  1.00 40.57      C
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ATOM    191  CD1 PHE B 282      11.720 -41.074 -12.130  1.00 41.80      C
ATOM    192  CD2 PHE B 282      11.590 -42.886 -13.689  1.00 41.65      C
ATOM    193  CE1 PHE B 282      10.975 -41.806 -11.209  1.00 42.03      C
ATOM    194  CE2 PHE B 282      10.843 -43.628 -12.773  1.00 42.49      C
ATOM    195  CZ  PHE B 282      10.536 -43.085 -11.532  1.00 41.74      C
ATOM    196  N   GLN B 288      16.212 -45.321 -19.533  1.00 30.94      N
ATOM    197  CA  GLN B 288      15.622 -44.804 -20.755  1.00 30.77      C
ATOM    198  C   GLN B 288      15.783 -43.291 -20.885  1.00 29.70      C
ATOM    199  O   GLN B 288      16.268 -42.801 -21.902  1.00 29.79      O
ATOM    200  CB  GLN B 288      14.143 -45.158 -20.810  1.00 30.59      C
ATOM    201  CG  GLN B 288      13.473 -44.772 -22.109  1.00 29.73      C
ATOM    202  CD  GLN B 288      11.981 -44.971 -22.044  1.00 28.04      C
ATOM    203  OE1 GLN B 288      11.294 -44.295 -21.279  1.00 29.59      O
ATOM    204  NE2 GLN B 288      11.468 -45.905 -22.838  1.00 26.98      N
ATOM    205  N   GLN B 289      15.378 -42.554 -19.857  1.00 29.38      N
ATOM    206  CA  GLN B 289      15.474 -41.099 -19.904  1.00 29.46      C
ATOM    207  C   GLN B 289      16.906 -40.613 -20.005  1.00 29.36      C
ATOM    208  O   GLN B 289      17.173 -39.557 -20.585  1.00 29.12      O
ATOM    209  CB  GLN B 289      14.772 -40.472 -18.700  1.00 29.25      C
ATOM    210  CG  GLN B 289      13.265 -40.416 -18.883  1.00 29.32      C
ATOM    211  CD  GLN B 289      12.575 -39.585 -17.826  1.00 29.84      C
ATOM    212  OE1 GLN B 289      13.191 -38.728 -17.188  1.00 29.52      O
ATOM    213  NE2 GLN B 289      11.281 -39.821 -17.647  1.00 28.95      N
ATOM    214  N   TYR B 290      17.835 -41.374 -19.442  1.00 28.95      N
ATOM    215  CA  TYR B 290      19.228 -40.984 -19.550  1.00 29.55      C
ATOM    216  C   TYR B 290      19.593 -41.042 -21.032  1.00 28.80      C
ATOM    217  O   TYR B 290      20.192 -40.113 -21.567  1.00 29.22      O
ATOM    218  CB  TYR B 290      20.136 -41.934 -18.768  1.00 31.40      C
ATOM    219  CG  TYR B 290      21.587 -41.780 -19.148  1.00 33.37      C
ATOM    220  CD1 TYR B 290      22.332 -40.682 -18.717  1.00 34.57      C
ATOM    221  CD2 TYR B 290      22.192 -42.684 -20.017  1.00 34.90      C
ATOM    222  CE1 TYR B 290      23.644 -40.490 -19.148  1.00 35.97      C
ATOM    223  CE2 TYR B 290      23.497 -42.500 -20.453  1.00 36.03      C
ATOM    224  CZ  TYR B 290      24.214 -41.402 -20.019  1.00 36.29      C
ATOM    225  OH  TYR B 290      25.499 -41.215 -20.475  1.00 39.44      O
ATOM    226  N   ASN B 292      17.658 -40.779 -23.508  1.00 25.52      N
ATOM    227  CA  ASN B 292      16.902 -39.784 -24.270  1.00 26.06      C
ATOM    228  C   ASN B 292      17.605 -38.427 -24.258  1.00 25.99      C
ATOM    229  O   ASN B 292      17.566 -37.687 -25.244  1.00 26.18      O
ATOM    230  CB  ASN B 292      15.484 -39.599 -23.709  1.00 24.78      C
ATOM    231  CG  ASN B 292      14.590 -40.811 -23.928  1.00 24.46      C
ATOM    232  OD1 ASN B 292      14.842 -41.641 -24.798  1.00 25.33      O
ATOM    233  ND2 ASN B 292      13.523 -40.900 -23.146  1.00 23.83      N
ATOM    234  N   ALA B 293      18.242 -38.105 -23.139  1.00 25.66      N
ATOM    235  CA  ALA B 293      18.926 -36.822 -22.979  1.00 25.69      C
ATOM    236  C   ALA B 293      20.346 -36.800 -23.521  1.00 25.67      C
ATOM    237  O   ALA B 293      20.855 -35.743 -23.902  1.00 25.52      O
ATOM    238  CB  ALA B 293      18.940 -36.422 -21.506  1.00 24.17      C
ATOM    239  N   LEU B 296      21.375 -34.703 -26.688  1.00 25.66      N
ATOM    240  CA  LEU B 296      21.521 -33.265 -26.481  1.00 25.42      C
ATOM    241  C   LEU B 296      22.784 -32.935 -25.688  1.00 26.07      C
ATOM    242  O   LEU B 296      23.435 -31.917 -25.944  1.00 25.26      O
ATOM    243  CB  LEU B 296      20.283 -32.685 -25.779  1.00 24.45      C
ATOM    244  CG  LEU B 296      19.066 -32.458 -26.679  1.00 25.59      C
ATOM    245  CD1 LEU B 296      17.968 -31.718 -25.911  1.00 23.56      C
ATOM    246  CD2 LEU B 296      19.496 -31.630 -27.893  1.00 25.87      C
ATOM    247  N   ALA B 302      23.066 -29.504 -23.507  1.00 20.94      N
ATOM    248  CA  ALA B 302      22.516 -29.770 -22.186  1.00 21.78      C
ATOM    249  C   ALA B 302      23.503 -30.507 -21.288  1.00 22.69      C
ATOM    250  O   ALA B 302      24.561 -30.948 -21.739  1.00 22.25      O
ATOM    251  CB  ALA B 302      21.243 -30.595 -22.327  1.00 20.10      C
ATOM    252  N   LYS B 303      23.156 -30.613 -20.009  1.00 24.62      N
ATOM    253  CA  LYS B 303      23.979 -31.340 -19.048  1.00 25.86      C
ATOM    254  C   LYS B 303      23.083 -32.319 -18.302  1.00 26.41      C
ATOM    255  O   LYS B 303      22.015 -31.948 -17.802  1.00 25.76      O
ATOM    256  CB  LYS B 303      24.632 -30.401 -18.036  1.00 27.85      C
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ATOM    257  CG  LYS B 303      25.466 -31.146 -16.986  1.00 29.37      C
ATOM    258  CD  LYS B 303      26.150 -30.186 -16.025  1.00 32.41      C
ATOM    259  CE  LYS B 303      27.083 -30.912 -15.056  1.00 33.22      C
ATOM    260  NZ  LYS B 303      27.827 -29.952 -14.181  1.00 33.62      N
ATOM    261  N   ILE B 304      23.520 -33.570 -18.234  1.00 25.65      N
ATOM    262  CA  ILE B 304      22.753 -34.598 -17.550  1.00 27.17      C
ATOM    263  C   ILE B 304      23.308 -34.855 -16.160  1.00 27.00      C
ATOM    264  O   ILE B 304      24.511 -35.012 -15.986  1.00 27.46      O
ATOM    265  CB  ILE B 304      22.786 -35.946 -18.316  1.00 27.06      C
ATOM    266  CG1 ILE B 304      22.242 -35.769 -19.733  1.00 27.61      C
ATOM    267  CG2 ILE B 304      21.977 -36.996 -17.555  1.00 28.49      C
ATOM    268  CD1 ILE B 304      22.380 -37.009 -20.599  1.00 27.05      C
ATOM    269  N   ILE B 305      22.428 -34.869 -15.168  1.00 27.22      N
ATOM    270  CA  ILE B 305      22.843 -35.178 -13.813  1.00 29.01      C
ATOM    271  C   ILE B 305      21.934 -36.302 -13.351  1.00 29.64      C
ATOM    272  O   ILE B 305      20.806 -36.067 -12.932  1.00 29.25      O
ATOM    273  CB  ILE B 305      22.713 -33.977 -12.858  1.00 28.91      C
ATOM    274  CG1 ILE B 305      23.660 -32.855 -13.299  1.00 29.51      C
ATOM    275  CG2 ILE B 305      23.063 -34.416 -11.432  1.00 30.98      C
ATOM    276  CD1 ILE B 305      23.674 -31.653 -12.367  1.00 29.43      C
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TABLE 5 ATOMIC COORDINATES OF ACCEPTOR BINDING SITE

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REMARK    4 1MUR COMPLIES WITH FORMAT V. 2.0, 11-MAY-2000
ATOM      1  N   MET B  12      -0.734 -48.902 -33.817  1.00 23.68      N
ATOM      2  CA  MET B  12      -0.523 -49.707 -32.613  1.00 24.54      C
ATOM      3  C   MET B  12       0.361 -48.840 -31.720  1.00 25.31      C
ATOM      4  O   MET B  12       1.546 -48.645 -32.006  1.00 23.88      O
ATOM      5  CB  MET B  12       0.192 -51.019 -32.971  1.00 24.28      C
ATOM      6  CG  MET B  12      -0.402 -51.726 -34.188  1.00 25.19      C
ATOM      7  SD  MET B  12       0.399 -53.284 -34.669  1.00 26.54      S
ATOM      8  CE  MET B  12       1.990 -52.691 -35.289  1.00 22.99      C
ATOM      9  N   ALA B  13      -0.224 -48.292 -30.657  1.00 27.08      N
ATOM     10  CA  ALA B  13       0.508 -47.410 -29.752  1.00 29.43      C
ATOM     11  C   ALA B  13      -0.239 -47.192 -28.436  1.00 31.80      C
ATOM     12  O   ALA B  13      -1.143 -46.350 -28.352  1.00 32.16      O
ATOM     13  CB  ALA B  13       0.747 -46.074 -30.429  1.00 28.82      C
ATOM     14  N   GLY B  14       0.150 -47.934 -27.405  1.00 32.46      N
ATOM     15  CA  GLY B  14      -0.513 -47.804 -26.120  1.00 33.82      C
ATOM     16  C   GLY B  14      -0.107 -46.595 -25.299  1.00 34.82      C
ATOM     17  O   GLY B  14       0.975 -46.040 -25.479  1.00 35.47      O
ATOM     18  N   GLY B  15      -0.986 -46.188 -24.385  1.00 35.56      N
ATOM     19  CA  GLY B  15      -0.700 -45.047 -23.536  1.00 36.08      C
ATOM     20  C   GLY B  15       0.539 -45.254 -22.683  1.00 36.84      C
ATOM     21  O   GLY B  15       1.293 -44.311 -22.426  1.00 36.03      O
ATOM     22  N   THR B  16       0.755 -46.488 -22.240  1.00 36.65      N
ATOM     23  CA  THR B  16       1.920 -46.787 -21.421  1.00 38.51      C
ATOM     24  C   THR B  16       3.158 -46.497 -22.264  1.00 38.35      C
ATOM     25  O   THR B  16       3.191 -46.798 -23.460  1.00 39.90      O
ATOM     26  CB  THR B  16       1.926 -48.258 -20.974  1.00 38.51      C
ATOM     27  OG1 THR B  16       0.686 -48.558 -20.321  1.00 38.39      O
ATOM     28  CG2 THR B  16       3.075 -48.518 -20.005  1.00 39.11      C
ATOM     29  N   GLY B  17       4.168 -45.897 -21.649  1.00 37.68      N
ATOM     30  CA  GLY B  17       5.367 -45.567 -22.392  1.00 36.57      C
ATOM     31  C   GLY B  17       5.161 -44.303 -23.211  1.00 35.56      C
ATOM     32  O   GLY B  17       6.079 -43.843 -23.890  1.00 35.03      O
ATOM     33  N   GLY B  18       3.949 -43.752 -23.150  1.00 33.83      N
ATOM     34  CA  GLY B  18       3.631 -42.529 -23.872  1.00 33.48      C
ATOM     35  C   GLY B  18       3.825 -42.593 -25.378  1.00 33.12      C
ATOM     36  O   GLY B  18       4.345 -41.650 -25.984  1.00 35.38      O
ATOM     37  N   HIS B  19       3.416 -43.699 -25.988  1.00 30.26      N
ATOM     38  CA  HIS B  19       3.548 -43.865 -27.435  1.00 28.22      C
ATOM     39  C   HIS B  19       2.280 -43.370 -28.144  1.00 27.91      C
ATOM     40  O   HIS B  19       2.300 -43.049 -29.337  1.00 26.91      O
ATOM     41  CB  HIS B  19       3.772 -45.349 -27.779  1.00 25.81      C
ATOM     42  CG  HIS B  19       4.957 -45.966 -27.094  1.00 25.35      C
ATOM     43  ND1 HIS B  19       4.845 -47.025 -26.217  1.00 24.57      N
ATOM     44  CD2 HIS B  19       6.281 -45.694 -27.184  1.00 24.18      C
ATOM     45  CE1 HIS B  19       6.046 -47.380 -25.798  1.00 23.08      C
ATOM     46  NE2 HIS B  19       6.936 -46.589 -26.369  1.00 25.51      N
ATOM     47  N   VAL B  20       1.180 -43.310 -27.402  1.00 27.65      N
ATOM     48  CA  VAL B  20      -0.098 -42.894 -27.965  1.00 27.77      C
ATOM     49  C   VAL B  20      -0.140 -41.452 -28.470  1.00 27.57      C
ATOM     50  O   VAL B  20      -0.771 -41.172 -29.486  1.00 27.12      O
ATOM     51  CB  VAL B  20      -1.248 -43.080 -26.942  1.00 28.57      C
ATOM     52  CG1 VAL B  20      -1.082 -42.114 -25.787  1.00 30.03      C
ATOM     53  CG2 VAL B  20      -2.602 -42.873 -27.631  1.00 26.82      C
ATOM     54  N   LEU B  40      -5.323 -50.004 -32.549  1.00 25.21      N
ATOM     55  CA  LEU B  40      -5.200 -51.364 -32.026  1.00 24.71      C
ATOM     56  C   LEU B  40      -4.535 -51.235 -30.655  1.00 23.33      C
ATOM     57  O   LEU B  40      -3.387 -50.824 -30.563  1.00 23.43      O
ATOM     58  CB  LEU B  40      -4.326 -52.221 -32.952  1.00 25.21      C
ATOM     59  CG  LEU B  40      -4.416 -53.754 -32.868  1.00 26.95      C
ATOM     60  CD1 LEU B  40      -3.037 -54.334 -32.571  1.00 27.63      C
ATOM     61  CD2 LEU B  40      -5.421 -54.179 -31.817  1.00 26.69      C
ATOM     62  N   GLU B  47      -4.976 -45.941 -23.678  1.00 32.85      N
ATOM     63  CA  GLU B  47      -5.458 -45.655 -25.029  1.00 31.79      C
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ATOM     64  C   GLU B  47      -6.938 -46.017 -25.191  1.00 31.81      C
ATOM     65  O   GLU B  47      -7.626 -45.476 -26.055  1.00 31.31      O
ATOM     66  CB  GLU B  47      -4.624 -46.402 -26.080  1.00 30.62      C
ATOM     67  CG  GLU B  47      -4.755 -47.922 -26.051  1.00 29.85      C
ATOM     68  CD  GLU B  47      -3.793 -48.597 -25.082  1.00 29.78      C
ATOM     69  OE1 GLU B  47      -3.188 -47.895 -24.247  1.00 28.76      O
ATOM     70  OE2 GLU B  47      -3.649 -49.840 -25.156  1.00 29.01      O
ATOM     71  N   ILE B  63      -3.428 -59.342 -24.313  1.00 30.07      N
ATOM     72  CA  ILE B  63      -2.036 -59.770 -24.231  1.00 31.38      C
ATOM     73  C   ILE B  63      -1.623 -59.981 -22.775  1.00 33.08      C
ATOM     74  O   ILE B  63      -0.444 -59.872 -22.430  1.00 33.21      O
ATOM     75  CB  ILE B  63      -1.081 -58.745 -24.883  1.00 30.06      C
ATOM     76  CG1 ILE B  63      -1.143 -57.411 -24.137  1.00 29.94      C
ATOM     77  CG2 ILE B  63      -1.442 -58.567 -26.353  1.00 30.41      C
ATOM     78  CD1 ILE B  63      -0.128 -56.384 -24.632  1.00 29.62      C
ATOM     79  N   ARG B  67       2.953 -59.185 -21.440  1.00 31.54      N
ATOM     80  CA  ARG B  67       3.671 -57.928 -21.277  1.00 30.90      C
ATOM     81  C   ARG B  67       5.071 -58.142 -20.713  1.00 29.99      C
ATOM     82  O   ARG B  67       5.294 -59.034 -19.889  1.00 28.67      O
ATOM     83  CB  ARG B  67       2.888 -56.984 -20.363  1.00 32.28      C
ATOM     84  CG  ARG B  67       1.540 -56.576 -20.913  1.00 34.65      C
ATOM     85  CD  ARG B  67       0.926 -55.440 -20.097  1.00 36.69      C
ATOM     86  NE  ARG B  67      -0.259 -54.889 -20.748  1.00 38.28      N
ATOM     87  CZ  ARG B  67      -1.425 -55.519 -20.853  1.00 39.05      C
ATOM     88  NH1 ARG B  67      -1.583 -56.734 -20.341  1.00 39.61      N
ATOM     89  NH2 ARG B  67      -2.434 -54.935 -21.487  1.00 39.52      N
ATOM     90  N   GLY B  68       6.014 -57.321 -21.165  1.00 27.75      N
ATOM     91  CA  GLY B  68       7.380 -57.427 -20.685  1.00 26.79      C
ATOM     92  C   GLY B  68       8.166 -58.579 -21.280  1.00 25.41      C
ATOM     93  O   GLY B  68       9.326 -58.779 -20.943  1.00 26.04      O
ATOM     94  N   GLY B 102       3.556 -48.986 -35.936  1.00 20.96      N
ATOM     95  CA  GLY B 102       3.796 -49.357 -34.549  1.00 19.23      C
ATOM     96  C   GLY B 102       4.655 -48.282 -33.918  1.00 18.45      C
ATOM     97  O   GLY B 102       5.765 -48.016 -34.381  1.00 18.70      O
ATOM     98  N   MET B 103       4.155 -47.660 -32.857  1.00 18.01      N
ATOM     99  CA  MET B 103       4.892 -46.597 -32.191  1.00 18.93      C
ATOM    100  C   MET B 103       5.612 -47.128 -30.957  1.00 18.98      C
ATOM    101  O   MET B 103       6.134 -46.357 -30.158  1.00 17.96      O
ATOM    102  CB  MET B 103       3.928 -45.477 -31.781  1.00 20.02      C
ATOM    103  CG  MET B 103       3.121 -44.888 -32.944  1.00 21.61      C
ATOM    104  SD  MET B 103       4.212 -44.135 -34.157  1.00 23.45      S
ATOM    105  CE  MET B 103       4.718 -42.680 -33.271  1.00 21.40      C
ATOM    106  N   GLY B 104       5.640 -48.450 -30.827  1.00 21.56      N
ATOM    107  CA  GLY B 104       6.275 -49.080 -29.686  1.00 21.89      C
ATOM    108  C   GLY B 104       5.192 -49.614 -28.764  1.00 23.28      C
ATOM    109  O   GLY B 104       4.009 -49.353 -28.980  1.00 22.50      O
ATOM    110  N   GLY B 105       5.583 -50.364 -27.741  1.00 23.01      N
ATOM    111  CA  GLY B 105       4.593 -50.905 -26.827  1.00 23.54      C
ATOM    112  C   GLY B 105       4.358 -52.380 -27.078  1.00 23.17      C
ATOM    113  O   GLY B 105       4.449 -52.844 -28.214  1.00 22.69      O
ATOM    114  N   TYR B 106       4.018 -53.118 -26.026  1.00 22.87      N
ATOM    115  CA  TYR B 106       3.818 -54.554 -26.159  1.00 22.37      C
ATOM    116  C   TYR B 106       2.719 -55.018 -27.100  1.00 20.52      C
ATOM    117  O   TYR B 106       2.867 -56.052 -27.746  1.00 20.50      O
ATOM    118  CB  TYR B 106       3.632 -55.181 -24.774  1.00 25.08      C
ATOM    119  CG  TYR B 106       4.864 -55.008 -23.929  1.00 28.19      C
ATOM    120  CD1 TYR B 106       4.869 -54.153 -22.830  1.00 31.96      C
ATOM    121  CD2 TYR B 106       6.058 -55.631 -24.282  1.00 31.27      C
ATOM    122  CE1 TYR B 106       6.043 -53.915 -22.108  1.00 33.13      C
ATOM    123  CE2 TYR B 106       7.234 -55.400 -23.569  1.00 32.27      C
ATOM    124  CZ  TYR B 106       7.219 -54.541 -22.487  1.00 33.19      C
ATOM    125  OH  TYR B 106       8.388 -54.291 -21.802  1.00 35.95      O
ATOM    126  N   VAL B 107       1.628 -54.270 -27.205  1.00 19.06      N
ATOM    127  CA  VAL B 107       0.557 -54.694 -28.099  1.00 18.06      C
ATOM    128  C   VAL B 107       1.015 -54.743 -29.559  1.00 17.45      C
ATOM    129  O   VAL B 107       0.502 -55.536 -30.346  1.00 16.99      O
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ATOM    130  CB  VAL B 107      -0.690 -53.774 -27.978  1.00 20.95      C
ATOM    131  CG1 VAL B 107      -0.407 -52.407 -28.589  1.00 21.39      C
ATOM    132  CG2 VAL B 107      -1.879 -54.433 -28.658  1.00 21.30      C
ATOM    133  N   SER B 108       1.991 -53.916 -29.918  1.00 17.96      N
ATOM    134  CA  SER B 108       2.488 -53.892 -31.290  1.00 19.67      C
ATOM    135  C   SER B 108       3.197 -55.187 -31.694  1.00 20.38      C
ATOM    136  O   SER B 108       3.385 -55.449 -32.884  1.00 21.25      O
ATOM    137  CB  SER B 108       3.424 -52.691 -31.508  1.00 19.56      C
ATOM    138  OG  SER B 108       4.666 -52.824 -30.837  1.00 19.63      O
ATOM    139  N   GLY B 109       3.595 -55.995 -30.710  1.00 19.59      N
ATOM    140  CA  GLY B 109       4.251 -57.256 -31.023  1.00 20.03      C
ATOM    141  C   GLY B 109       3.311 -58.170 -31.792  1.00 19.61      C
ATOM    142  O   GLY B 109       3.579 -58.517 -32.940  1.00 19.24      O
ATOM    143  N   PRO B 110       2.206 -58.606 -31.173  1.00 19.20      N
ATOM    144  CA  PRO B 110       1.251 -59.478 -31.855  1.00 18.99      C
ATOM    145  C   PRO B 110       0.651 -58.761 -33.075  1.00 19.22      C
ATOM    146  O   PRO B 110       0.406 -59.371 -34.116  1.00 17.13      O
ATOM    147  CB  PRO B 110       0.198 -59.737 -30.778  1.00 20.41      C
ATOM    148  CG  PRO B 110       0.998 -59.720 -29.515  1.00 19.81      C
ATOM    149  CD  PRO B 110       1.914 -58.528 -29.729  1.00 19.94      C
ATOM    150  N   HIS B 125       8.182 -46.638 -35.447  1.00 21.40      N
ATOM    151  CA  HIS B 125       8.814 -45.413 -34.981  1.00 21.42      C
ATOM    152  C   HIS B 125       9.196 -45.642 -33.519  1.00 21.70      C
ATOM    153  O   HIS B 125       8.378 -46.117 -32.725  1.00 19.81      O
ATOM    154  CB  HIS B 125       7.858 -44.218 -35.067  1.00 21.57      C
ATOM    155  CG  HIS B 125       8.432 -42.948 -34.511  1.00 23.73      C
ATOM    156  ND1 HIS B 125       9.274 -42.127 -35.236  1.00 26.23      N
ATOM    157  CD2 HIS B 125       8.300 -42.368 -33.295  1.00 22.15      C
ATOM    158  CE1 HIS B 125       9.631 -41.095 -34.490  1.00 24.20      C
ATOM    159  NE2 HIS B 125       9.054 -41.218 -33.307  1.00 26.07      N
ATOM    160  N   GLU B 126      10.444 -45.332 -33.186  1.00 21.20      N
ATOM    161  CA  GLU B 126      10.947 -45.452 -31.817  1.00 22.15      C
ATOM    162  C   GLU B 126      11.205 -44.027 -31.326  1.00 21.93      C
ATOM    163  O   GLU B 126      12.016 -43.300 -31.908  1.00 21.33      O
ATOM    164  CB  GLU B 126      12.252 -46.246 -31.790  1.00 21.99      C
ATOM    165  CG  GLU B 126      12.958 -46.206 -30.439  1.00 22.04      C
ATOM    166  CD  GLU B 126      12.119 -46.824 -29.338  1.00 21.43      C
ATOM    167  OE1 GLU B 126      11.767 -48.014 -29.471  1.00 21.92      O
ATOM    168  OE2 GLU B 126      11.807 -46.124 -28.349  1.00 21.08      O
ATOM    169  N   GLN B 127      10.520 -43.624 -30.259  1.00 22.62      N
ATOM    170  CA  GLN B 127      10.682 -42.270 -29.735  1.00 22.81      C
ATOM    171  C   GLN B 127      11.874 -42.087 -28.809  1.00 22.39      C
ATOM    172  O   GLN B 127      12.399 -40.976 -28.682  1.00 22.43      O
ATOM    173  CB  GLN B 127       9.414 -41.814 -28.989  1.00 23.56      C
ATOM    174  CG  GLN B 127       8.147 -41.783 -29.830  1.00 24.46      C
ATOM    175  CD  GLN B 127       7.312 -43.041 -29.687  1.00 25.85      C
ATOM    176  OE1 GLN B 127       6.842 -43.366 -28.591  1.00 23.78      O
ATOM    177  NE2 GLN B 127       7.119 -43.758 -30.797  1.00 24.91      N
ATOM    178  N   ASN B 128      12.314 -43.173 -28.177  1.00 22.35      N
ATOM    179  CA  ASN B 128      13.406 -43.097 -27.216  1.00 22.96      C
ATOM    180  C   ASN B 128      14.824 -43.314 -27.742  1.00 23.87      C
ATOM    181  O   ASN B 128      15.026 -43.856 -28.830  1.00 24.05      O
ATOM    182  CB  ASN B 128      13.136 -44.080 -26.064  1.00 22.85      C
ATOM    183  CG  ASN B 128      11.742 -43.919 -25.474  1.00 23.25      C
ATOM    184  OD1 ASN B 128      10.804 -44.632 -25.848  1.00 26.04      O
ATOM    185  ND2 ASN B 128      11.597 -42.975 -24.556  1.00 22.68      N
ATOM    186  N   GLY B 132      12.851 -49.814 -27.506  1.00 24.52      N
ATOM    187  CA  GLY B 132      12.007 -50.532 -26.568  1.00 24.05      C
ATOM    188  C   GLY B 132      12.150 -52.019 -26.831  1.00 23.35      C
ATOM    189  O   GLY B 132      12.582 -52.419 -27.904  1.00 22.89      O
ATOM    190  N   LEU B 133      11.788 -52.846 -25.860  1.00 23.38      N
ATOM    191  CA  LEU B 133      11.903 -54.293 -26.020  1.00 24.54      C
ATOM    192  C   LEU B 133      11.209 -54.833 -27.276  1.00 22.84      C
ATOM    193  O   LEU B 133      11.784 -55.619 -28.027  1.00 21.86      O
ATOM    194  CB  LEU B 133      11.328 -54.996 -24.786  1.00 25.48      C
ATOM    195  CG  LEU B 133      11.388 -56.527 -24.780  1.00 27.50      C
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ATOM    196  CD1 LEU B 133      12.840 -56.984 -24.866  1.00 28.69      C
ATOM    197  CD2 LEU B 133      10.735 -57.059 -23.509  1.00 28.04      C
ATOM    198  N   THR B 134       9.975 -54.401 -27.499  1.00 21.72      N
ATOM    199  CA  THR B 134       9.202 -54.860 -28.639  1.00 21.22      C
ATOM    200  C   THR B 134       9.693 -54.326 -29.986  1.00 20.62      C
ATOM    201  O   THR B 134       9.843 -55.091 -30.932  1.00 20.33      O
ATOM    202  CB  THR B 134       7.716 -54.509 -28.449  1.00 20.99      C
ATOM    203  OG1 THR B 134       7.257 -55.075 -27.210  1.00 20.94      O
ATOM    204  CG2 THR B 134       6.872 -55.073 -29.600  1.00 20.64      C
ATOM    205  N   ASN B 135       9.932 -53.021 -30.075  1.00 21.24      N
ATOM    206  CA  ASN B 135      10.407 -52.419 -31.324  1.00 20.50      C
ATOM    207  C   ASN B 135      11.724 -53.064 -31.767  1.00 20.78      C
ATOM    208  O   ASN B 135      11.945 -53.290 -32.953  1.00 20.41      O
ATOM    209  CB  ASN B 135      10.637 -50.911 -31.142  1.00 19.58      C
ATOM    210  CG  ASN B 135       9.457 -50.058 -31.597  1.00 19.93      C
ATOM    211  OD1 ASN B 135       9.454 -48.837 -31.390  1.00 21.78      O
ATOM    212  ND2 ASN B 135       8.467 -50.677 -32.219  1.00 17.21      N
ATOM    213  N   LEU B 138      10.741 -56.381 -33.386  1.00 21.61      N
ATOM    214  CA  LEU B 138       9.744 -56.188 -34.431  1.00 23.15      C
ATOM    215  C   LEU B 138      10.384 -55.558 -35.676  1.00 23.07      C
ATOM    216  O   LEU B 138       9.958 -55.801 -36.809  1.00 22.68      O
ATOM    217  CB  LEU B 138       8.618 -55.305 -33.886  1.00 23.87      C
ATOM    218  CG  LEU B 138       7.312 -55.155 -34.664  1.00 26.48      C
ATOM    219  CD1 LEU B 138       6.672 -56.508 -34.915  1.00 25.34      C
ATOM    220  CD2 LEU B 138       6.383 -54.267 -33.851  1.00 25.90      C
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TABLE 6 ATOMIC COORDINATES OF MEMBRANE ASSOCIATION SITE

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REMARK    4 1MUR COMPLIES WITH FORMAT V. 2.0, 11-MAY-2000
ATOM      1  N   MET B  12      -0.734 -48.902 -33.817  1.00 23.68      N
ATOM      2  CA  MET B  12      -0.523 -49.707 -32.613  1.00 24.54      C
ATOM      3  C   MET B  12       0.361 -48.840 -31.720  1.00 25.31      C
ATOM      4  O   MET B  12       1.546 -48.645 -32.006  1.00 23.88      O
ATOM      5  CB  MET B  12       0.192 -51.019 -32.971  1.00 24.28      C
ATOM      6  CG  MET B  12      -0.402 -51.726 -34.188  1.00 25.19      C
ATOM      7  SD  MET B  12       0.399 -53.284 -34.669  1.00 26.54      S
ATOM      8  CE  MET B  12       1.990 -52.691 -35.289  1.00 22.99      C
ATOM      9  N   LEU B  40      -5.323 -50.004 -32.549  1.00 25.21      N
ATOM     10  CA  LEU B  40      -5.200 -51.364 -32.026  1.00 24.71      C
ATOM     11  C   LEU B  40      -4.535 -51.235 -30.655  1.00 23.33      C
ATOM     12  O   LEU B  40      -3.387 -50.824 -30.563  1.00 23.43      O
ATOM     13  CB  LEU B  40      -4.326 -52.221 -32.952  1.00 25.21      C
ATOM     14  CG  LEU B  40      -4.416 -53.754 -32.868  1.00 26.95      C
ATOM     15  CD1 LEU B  40      -3.037 -54.334 -32.571  1.00 27.63      C
ATOM     16  CD2 LEU B  40      -5.421 -54.179 -31.817  1.00 26.69      C
ATOM     17  N   ILE B  61      -7.271 -56.229 -28.295  1.00 29.38      N
ATOM     18  CA  ILE B  61      -6.832 -57.616 -28.269  1.00 28.55      C
ATOM     19  C   ILE B  61      -6.344 -57.855 -26.848  1.00 29.13      C
ATOM     20  O   ILE B  61      -6.124 -56.906 -26.091  1.00 28.80      O
ATOM     21  CB  ILE B  61      -5.674 -57.923 -29.258  1.00 28.48      C
ATOM     22  CG1 ILE B  61      -4.422 -57.126 -28.892  1.00 26.70      C
ATOM     23  CG2 ILE B  61      -6.123 -57.650 -30.694  1.00 27.65      C
ATOM     24  CD1 ILE B  61      -3.177 -57.615 -29.638  1.00 27.03      C
ATOM     25  N   ARG B  62      -6.186 -59.116 -26.473  1.00 29.38      N
ATOM     26  CA  ARG B  62      -5.709 -59.416 -25.133  1.00 30.76      C
ATOM     27  C   ARG B  62      -4.274 -59.923 -25.156  1.00 29.32      C
ATOM     28  O   ARG B  62      -3.933 -60.809 -25.934  1.00 28.65      O
ATOM     29  CB  ARG B  62      -6.630 -60.447 -24.461  1.00 32.36      C
ATOM     30  CG  ARG B  62      -6.130 -60.955 -23.114  1.00 35.99      C
ATOM     31  CD  ARG B  62      -5.438 -59.859 -22.311  1.00 37.86      C
ATOM     32  NE  ARG B  62      -6.297 -58.718 -22.004  1.00 40.01      N
ATOM     33  CZ  ARG B  62      -5.840 -57.504 -21.711  1.00 39.09      C
ATOM     34  NH1 ARG B  62      -4.536 -57.275 -21.690  1.00 39.24      N
ATOM     35  NH2 ARG B  62      -6.686 -56.518 -21.439  1.00 40.03      N
ATOM     36  N   ILE B  63      -3.428 -59.342 -24.313  1.00 30.07      N
ATOM     37  CA  ILE B  63      -2.036 -59.770 -24.231  1.00 31.38      C
ATOM     38  C   ILE B  63      -1.623 -59.981 -22.775  1.00 33.08      C
ATOM     39  O   ILE B  63      -0.444 -59.872 -22.430  1.00 33.21      O
ATOM     40  CB  ILE B  63      -1.081 -58.745 -24.883  1.00 30.06      C
ATOM     41  CG1 ILE B  63      -1.143 -57.411 -24.137  1.00 29.94      C
ATOM     42  CG2 ILE B  63      -1.442 -58.567 -26.353  1.00 30.41      C
ATOM     43  CD1 ILE B  63      -0.128 -56.384 -24.632  1.00 29.62      C
ATOM     44  N   SER B  64      -2.603 -60.284 -21.927  1.00 35.38      N
ATOM     45  CA  SER B  64      -2.356 -60.520 -20.505  1.00 37.51      C
ATOM     46  C   SER B  64      -1.326 -61.622 -20.311  1.00 37.32      C
ATOM     47  O   SER B  64      -1.411 -62.682 -20.933  1.00 37.86      O
ATOM     48  CB  SER B  64      -3.652 -60.912 -19.792  1.00 38.82      C
ATOM     49  OG  SER B  64      -4.558 -59.823 -19.750  1.00 42.88      O
ATOM     50  N   GLY B  65      -0.356 -61.370 -19.441  1.00 37.81      N
ATOM     51  CA  GLY B  65       0.679 -62.355 -19.199  1.00 37.13      C
ATOM     52  C   GLY B  65       1.798 -62.283 -20.226  1.00 36.76      C
ATOM     53  O   GLY B  65       2.858 -62.889 -20.038  1.00 37.57      O
ATOM     54  N   LEU B  66       1.577 -61.539 -21.307  1.00 34.63      N
ATOM     55  CA  LEU B  66       2.591 -61.413 -22.355  1.00 33.17      C
ATOM     56  C   LEU B  66       3.414 -60.133 -22.246  1.00 32.72      C
ATOM     57  O   LEU B  66       4.451 -60.002 -22.893  1.00 33.13      O
ATOM     58  CB  LEU B  66       1.936 -61.470 -23.735  1.00 32.08      C
ATOM     59  CG  LEU B  66       1.162 -62.747 -24.061  1.00 32.52      C
ATOM     60  CD1 LEU B  66       0.563 -62.626 -25.445  1.00 31.38      C
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ATOM     61  CD2 LEU B  66       2.093 -63.957 -23.984  1.00 31.67      C
ATOM     62  N   ARG B  67       2.953 -59.185 -21.440  1.00 31.54      N
ATOM     63  CA  ARG B  67       3.671 -57.928 -21.277  1.00 30.90      C
ATOM     64  C   ARG B  67       5.071 -58.142 -20.713  1.00 29.99      C
ATOM     65  O   ARG B  67       5.294 -59.034 -19.889  1.00 28.67      O
ATOM     66  CB  ARG B  67       2.888 -56.984 -20.363  1.00 32.28      C
ATOM     67  CG  ARG B  67       1.540 -56.576 -20.913  1.00 34.65      C
ATOM     68  CD  ARG B  67       0.926 -55.440 -20.097  1.00 36.69      C
ATOM     69  NE  ARG B  67      -0.259 -54.889 -20.748  1.00 38.28      N
ATOM     70  CZ  ARG B  67      -1.425 -55.519 -20.853  1.00 39.05      C
ATOM     71  NH1 ARG B  67      -1.583 -56.734 -20.341  1.00 39.61      N
ATOM     72  NH2 ARG B  67      -2.434 -54.935 -21.487  1.00 39.52      N
ATOM     73  N   GLY B  68       6.014 -57.321 -21.165  1.00 27.75      N
ATOM     74  CA  GLY B  68       7.380 -57.427 -20.685  1.00 26.79      C
ATOM     75  C   GLY B  68       8.166 -58.579 -21.280  1.00 25.41      C
ATOM     76  O   GLY B  68       9.326 -58.779 -20.943  1.00 26.04      O
ATOM     77  N   LYS B  69       7.546 -59.342 -22.170  1.00 24.55      N
ATOM     78  CA  LYS B  69       8.238 -60.463 -22.796  1.00 23.93      C
ATOM     79  C   LYS B  69       8.825 -60.062 -24.142  1.00 23.32      C
ATOM     80  O   LYS B  69       8.151 -59.404 -24.944  1.00 21.96      O
ATOM     81  CB  LYS B  69       7.284 -61.641 -23.033  1.00 24.12      C
ATOM     82  CG  LYS B  69       6.757 -62.360 -21.794  1.00 25.08      C
ATOM     83  CD  LYS B  69       5.887 -63.553 -22.224  1.00 25.44      C
ATOM     84  CE  LYS B  69       5.357 -64.358 -21.035  1.00 28.31      C
ATOM     85  NZ  LYS B  69       6.468 -64.877 -20.175  1.00 29.71      N
ATOM     86  N   GLY B  70      10.075 -60.470 -24.374  1.00 22.48      N
ATOM     87  CA  GLY B  70      10.755 -60.229 -25.636  1.00 22.26      C
ATOM     88  C   GLY B  70      10.308 -61.337 -26.588  1.00 22.17      C
ATOM     89  O   GLY B  70       9.512 -62.183 -26.195  1.00 21.62      O
ATOM     90  N   ILE B  71      10.819 -61.373 -27.814  1.00 21.85      N
ATOM     91  CA  ILE B  71      10.357 -62.386 -28.762  1.00 23.55      C
ATOM     92  C   ILE B  71      10.616 -63.840 -28.359  1.00 23.88      C
ATOM     93  O   ILE B  71       9.775 -64.707 -28.592  1.00 21.66      O
ATOM     94  CB  ILE B  71      10.926 -62.142 -30.181  1.00 23.52      C
ATOM     95  CG1 ILE B  71      10.264 -63.096 -31.182  1.00 24.18      C
ATOM     96  CG2 ILE B  71      12.435 -62.375 -30.192  1.00 25.96      C
ATOM     97  CD1 ILE B  71       8.745 -62.981 -31.263  1.00 25.73      C
ATOM     98  N   LYS B  72      11.764 -64.119 -27.751  1.00 23.82      N
ATOM     99  CA  LYS B  72      12.038 -65.491 -27.343  1.00 24.92      C
ATOM    100  C   LYS B  72      11.068 -65.925 -26.245  1.00 23.73      C
ATOM    101  O   LYS B  72      10.592 -67.062 -26.245  1.00 24.08      O
ATOM    102  CB  LYS B  72      13.491 -65.634 -26.875  1.00 26.86      C
ATOM    103  CG  LYS B  72      14.496 -65.590 -28.019  1.00 31.29      C
ATOM    104  CD  LYS B  72      15.925 -65.791 -27.518  1.00 36.00      C
ATOM    105  CE  LYS B  72      16.926 -65.816 -28.671  1.00 38.82      C
ATOM    106  NZ  LYS B  72      18.342 -65.957 -28.192  1.00 41.21      N
ATOM    107  N   ALA B  73      10.765 -65.016 -25.322  1.00 21.62      N
ATOM    108  CA  ALA B  73       9.839 -65.306 -24.233  1.00 21.18      C
ATOM    109  C   ALA B  73       8.412 -65.454 -24.771  1.00 20.36      C
ATOM    110  O   ALA B  73       7.619 -66.250 -24.267  1.00 18.97      O
ATOM    111  CB  ALA B  73       9.895 -64.196 -23.187  1.00 22.25      C
ATOM    112  N   LEU B  74       8.076 -64.673 -25.791  1.00 20.23      N
ATOM    113  CA  LEU B  74       6.745 -64.762 -26.387  1.00 19.36      C
ATOM    114  C   LEU B  74       6.549 -66.110 -27.069  1.00 19.37      C
ATOM    115  O   LEU B  74       5.539 -66.779 -26.863  1.00 20.01      O
ATOM    116  CB  LEU B  74       6.540 -63.643 -27.417  1.00 18.42      C
ATOM    117  CG  LEU B  74       6.422 -62.208 -26.884  1.00 18.80      C
ATOM    118  CD1 LEU B  74       6.473 -61.197 -28.039  1.00 19.86      C
ATOM    119  CD2 LEU B  74       5.109 -62.071 -26.104  1.00 19.45      C
ATOM    120  N   ILE B  75       7.520 -66.507 -27.883  1.00 20.59      N
ATOM    121  CA  ILE B  75       7.434 -67.768 -28.601  1.00 21.18      C
ATOM    122  C   ILE B  75       7.488 -68.942 -27.624  1.00 21.20      C
ATOM    123  O   ILE B  75       7.125 -70.063 -27.979  1.00 21.59      O
ATOM    124  CB  ILE B  75       8.571 -67.896 -29.641  1.00 22.95      C
ATOM    125  CG1 ILE B  75       8.598 -66.657 -30.540  1.00 26.82      C
ATOM    126  CG2 ILE B  75       8.334 -69.108 -30.527  1.00 25.38      C
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ATOM	127	CD1	ILE	B	75	7.304	-66.442	-31.327	1.00	28.48	C
ATOM	128	N	ALA	B	76	7.940	-68.680	-26.399	1.00	20.49	N
ATOM	129	CA	ALA	B	76	7.996	-69.726	-25.374	1.00	21.72	C
ATOM	130	C	ALA	B	76	6.624	-69.904	-24.732	1.00	21.54	C
ATOM	131	O	ALA	B	76	6.441	-70.778	-23.875	1.00	20.75	O
ATOM	132	CB	ALA	B	76	9.026	-69.372	-24.305	1.00	21.92	C
ATOM	133	N	ALA	B	77	5.668	-69.066	-25.145	1.00	20.61	N
ATOM	134	CA	ALA	B	77	4.289	-69.121	-24.655	1.00	21.07	C
ATOM	135	C	ALA	B	77	3.383	-69.298	-25.881	1.00	21.69	C
ATOM	136	O	ALA	B	77	2.567	-68.430	-26.199	1.00	21.93	O
ATOM	137	CB	ALA	B	77	3.937	-67.830	-23.924	1.00	20.10	C
ATOM	138	N	PRO	B	78	3.507	-70.446	-26.564	1.00	22.38	N
ATOM	139	CA	PRO	B	78	2.772	-70.846	-27.771	1.00	20.95	C
ATOM	140	C	PRO	B	78	1.278	-70.535	-27.813	1.00	21.19	C
ATOM	141	O	PRO	B	78	0.789	-69.939	-28.776	1.00	19.68	O
ATOM	142	CB	PRO	B	78	3.027	-72.350	-27.861	1.00	22.21	C
ATOM	143	CG	PRO	B	78	4.288	-72.547	-27.117	1.00	24.07	C
ATOM	144	CD	PRO	B	78	4.211	-71.603	-25.976	1.00	21.89	C
ATOM	145	N	LEU	B	79	0.544	-70.961	-26.790	1.00	21.21	N
ATOM	146	CA	LEU	B	79	-0.896	-70.728	-26.783	1.00	21.32	C
ATOM	147	C	LEU	B	79	-1.275	-69.263	-26.707	1.00	21.17	C
ATOM	148	O	LEU	B	79	-2.125	-68.800	-27.481	1.00	20.44	O
ATOM	149	CB	LEU	B	79	-1.569	-71.476	-25.630	1.00	20.99	C
ATOM	150	CG	LEU	B	79	-1.397	-72.988	-25.617	1.00	22.40	C
ATOM	151	CD1	LEU	B	79	-2.504	-73.619	-24.772	1.00	22.01	C
ATOM	152	CD2	LEU	B	79	-1.438	-73.521	-27.021	1.00	23.82	C
ATOM	153	N	ARG	B	80	-0.656	-68.529	-25.788	1.00	20.91	N
ATOM	154	CA	ARG	B	80	-0.980	-67.115	-25.637	1.00	21.30	C
ATOM	155	C	ARG	B	80	-0.526	-66.233	-26.790	1.00	21.29	C
ATOM	156	O	ARG	B	80	-1.278	-65.355	-27.223	1.00	21.47	O
ATOM	157	CB	ARG	B	80	-0.444	-66.583	-24.312	1.00	22.12	C
ATOM	158	CG	ARG	B	80	-1.286	-67.051	-23.118	1.00	24.03	C
ATOM	159	CD	ARG	B	80	-0.610	-66.738	-21.807	1.00	23.42	C
ATOM	160	NE	ARG	B	80	0.581	-67.556	-21.610	1.00	24.59	N
ATOM	161	CZ	ARG	B	80	1.466	-67.351	-20.642	1.00	26.08	C
ATOM	162	NH1	ARG	B	80	1.290	-66.349	-19.787	1.00	26.92	N
ATOM	163	NH2	ARG	B	80	2.514	-68.152	-20.519	1.00	27.22	N
ATOM	164	N	ILE	B	81	0.683	-66.448	-27.303	1.00	19.29	N
ATOM	165	CA	ILE	B	81	1.113	-65.621	-28.421	1.00	19.47	C
ATOM	166	C	ILE	B	81	0.256	-65.937	-29.654	1.00	18.99	C
ATOM	167	O	ILE	B	81	-0.149	-65.028	-30.378	1.00	19.38	O
ATOM	168	CB	ILE	B	81	2.639	-65.793	-28.730	1.00	17.92	C
ATOM	169	CG1	ILE	B	81	3.067	-64.753	-29.769	1.00	18.63	C
ATOM	170	CG2	ILE	B	81	2.949	-67.200	-29.206	1.00	17.33	C
ATOM	171	CD1	ILE	B	81	2.746	-63.318	-29.346	1.00	17.46	C
ATOM	172	N	PHE	B	82	-0.056	-67.211	-29.880	1.00	19.39	N
ATOM	173	CA	PHE	B	82	-0.875	-67.582	-31.038	1.00	19.15	C
ATOM	174	C	PHE	B	82	-2.250	-66.931	-30.959	1.00	19.94	C
ATOM	175	O	PHE	B	82	-2.777	-66.444	-31.970	1.00	19.64	O
ATOM	176	CB	PHE	B	82	-1.057	-69.103	-31.136	1.00	19.27	C
ATOM	177	CG	PHE	B	82	-1.811	-69.548	-32.368	1.00	19.87	C
ATOM	178	CD1	PHE	B	82	-1.180	-69.602	-33.603	1.00	20.87	C
ATOM	179	CD2	PHE	B	82	-3.154	-69.898	-32.289	1.00	21.11	C
ATOM	180	CE1	PHE	B	82	-1.872	-70.002	-34.753	1.00	21.20	C
ATOM	181	CE2	PHE	B	82	-3.857	-70.297	-33.429	1.00	22.26	C
ATOM	182	CZ	PHE	B	82	-3.212	-70.349	-34.663	1.00	22.14	C
ATOM	183	N	ASN	B	83	-2.832	-66.923	-29.764	1.00	19.29	N
ATOM	184	CA	ASN	B	83	-4.150	-66.332	-29.577	1.00	20.90	C
ATOM	185	C	ASN	B	83	-4.178	-64.821	-29.812	1.00	20.83	C
ATOM	186	O	ASN	B	83	-5.086	-64.316	-30.472	1.00	21.92	O
ATOM	187	CB	ASN	B	83	-4.693	-66.641	-28.178	1.00	20.55	C
ATOM	188	CG	ASN	B	83	-6.158	-66.244	-28.028	1.00	22.79	C
ATOM	189	OD1	ASN	B	83	-6.505	-65.374	-27.229	1.00	25.14	O
ATOM	190	ND2	ASN	B	83	-7.018	-66.877	-28.807	1.00	20.47	N
ATOM	191	N	ALA	B	84	-3.203	-64.092	-29.275	1.00	19.74	N
ATOM	192	CA	ALA	B	84	-3.177	-62.647	-29.484	1.00	19.30	C

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ATOM    193  C   ALA B  84      -2.967 -62.380 -30.981  1.00 19.94      C
ATOM    194  O   ALA B  84      -3.561 -61.459 -31.552  1.00 19.69      O
ATOM    195  CB  ALA B  84      -2.060 -62.008 -28.662  1.00 18.59      C
ATOM    196  N   TRP B  85      -2.118 -63.197 -31.603  1.00 19.77      N
ATOM    197  CA  TRP B  85      -1.820 -63.111 -33.032  1.00 20.56      C
ATOM    198  C   TRP B  85      -3.090 -63.354 -33.865  1.00 21.76      C
ATOM    199  O   TRP B  85      -3.339 -62.658 -34.859  1.00 20.40      O
ATOM    200  CB  TRP B  85      -0.754 -64.148 -33.396  1.00 21.46      C
ATOM    201  CG  TRP B  85      -0.365 -64.167 -34.856  1.00 23.00      C
ATOM    202  CD1 TRP B  85       0.301 -63.189 -35.548  1.00 23.17      C
ATOM    203  CD2 TRP B  85      -0.588 -65.232 -35.785  1.00 23.69      C
ATOM    204  NE1 TRP B  85       0.509 -63.585 -36.848  1.00 24.28      N
ATOM    205  CE2 TRP B  85      -0.024 -64.835 -37.022  1.00 24.14      C
ATOM    206  CE3 TRP B  85      -1.206 -66.486 -35.693  1.00 24.79      C
ATOM    207  CZ2 TRP B  85      -0.060 -65.650 -38.160  1.00 24.90      C
ATOM    208  CZ3 TRP B  85      -1.243 -67.299 -36.827  1.00 25.45      C
ATOM    209  CH2 TRP B  85      -0.671 -66.875 -38.045  1.00 25.15      C
ATOM    210  N   ARG B  86      -3.885 -64.346 -33.467  1.00 22.03      N
ATOM    211  CA  ARG B  86      -5.140 -64.660 -34.166  1.00 23.28      C
ATOM    212  C   ARG B  86      -6.151 -63.517 -34.007  1.00 22.98      C
ATOM    213  O   ARG B  86      -6.890 -63.195 -34.942  1.00 21.37      O
ATOM    214  CB  ARG B  86      -5.754 -65.965 -33.623  1.00 24.72      C
ATOM    215  CG  ARG B  86      -4.999 -67.236 -34.021  1.00 27.21      C
ATOM    216  CD  ARG B  86      -5.368 -67.725 -35.418  1.00 29.60      C
ATOM    217  NE  ARG B  86      -6.626 -68.477 -35.422  1.00 31.45      N
ATOM    218  CZ  ARG B  86      -7.185 -69.004 -36.508  1.00 31.37      C
ATOM    219  NH1 ARG B  86      -6.607 -68.862 -37.696  1.00 32.19      N
ATOM    220  NH2 ARG B  86      -8.314 -69.694 -36.405  1.00 31.39      N
ATOM    221  N   GLN B  87      -6.190 -62.916 -32.821  1.00 22.90      N
ATOM    222  CA  GLN B  87      -7.101 -61.802 -32.567  1.00 24.07      C
ATOM    223  C   GLN B  87      -6.738 -60.618 -33.457  1.00 23.85      C
ATOM    224  O   GLN B  87      -7.613 -60.012 -34.077  1.00 24.02      O
ATOM    225  CB  GLN B  87      -7.046 -61.382 -31.097  1.00 24.33      C
ATOM    226  CG  GLN B  87      -7.873 -62.280 -30.187  1.00 27.24      C
ATOM    227  CD  GLN B  87      -7.720 -61.943 -28.723  1.00 28.81      C
ATOM    228  OE1 GLN B  87      -8.567 -62.296 -27.908  1.00 33.25      O
ATOM    229  NE2 GLN B  87      -6.632 -61.275 -28.375  1.00 29.95      N
ATOM    230  N   ALA B  88      -5.449 -60.293 -33.521  1.00 23.39      N
ATOM    231  CA  ALA B  88      -4.996 -59.183 -34.355  1.00 23.78      C
ATOM    232  C   ALA B  88      -5.257 -59.485 -35.831  1.00 24.73      C
ATOM    233  O   ALA B  88      -5.655 -58.595 -36.592  1.00 24.72      O
ATOM    234  CB  ALA B  88      -3.508 -58.909 -34.116  1.00 23.33      C
ATOM    235  N   ARG B  89      -5.038 -60.735 -36.244  1.00 24.26      N
ATOM    236  CA  ARG B  89      -5.285 -61.111 -37.636  1.00 24.94      C
ATOM    237  C   ARG B  89      -6.752 -60.909 -38.013  1.00 25.29      C
ATOM    238  O   ARG B  89      -7.056 -60.420 -39.104  1.00 24.27      O
ATOM    239  CB  ARG B  89      -4.904 -62.575 -37.893  1.00 25.14      C
ATOM    240  CG  ARG B  89      -3.461 -62.774 -38.353  1.00 24.54      C
ATOM    241  CD  ARG B  89      -3.142 -64.253 -38.510  1.00 25.50      C
ATOM    242  NE  ARG B  89      -3.809 -64.901 -39.641  1.00 24.93      N
ATOM    243  CZ  ARG B  89      -3.329 -64.930 -40.882  1.00 25.90      C
ATOM    244  NH1 ARG B  89      -2.178 -64.336 -41.170  1.00 25.98      N
ATOM    245  NH2 ARG B  89      -3.979 -65.596 -41.831  1.00 26.36      N
ATOM    246  N   GLY B 105       5.583 -50.364 -27.741  1.00 23.01      N
ATOM    247  CA  GLY B 105       4.593 -50.905 -26.827  1.00 23.54      C
ATOM    248  C   GLY B 105       4.358 -52.380 -27.078  1.00 23.17      C
ATOM    249  O   GLY B 105       4.449 -52.844 -28.214  1.00 22.69      O
ATOM    250  N   TYR B 106       4.018 -53.118 -26.026  1.00 22.87      N
ATOM    251  CA  TYR B 106       3.818 -54.554 -26.159  1.00 22.37      C
ATOM    252  C   TYR B 106       2.719 -55.018 -27.100  1.00 20.52      C
ATOM    253  O   TYR B 106       2.867 -56.052 -27.746  1.00 20.50      O
ATOM    254  CB  TYR B 106       3.632 -55.181 -24.774  1.00 25.08      C
ATOM    255  CG  TYR B 106       4.864 -55.008 -23.929  1.00 28.19      C
ATOM    256  CD1 TYR B 106       4.869 -54.153 -22.830  1.00 31.96      C
ATOM    257  CD2 TYR B 106       6.058 -55.631 -24.282  1.00 31.27      C
ATOM    258  CE1 TYR B 106       6.043 -53.915 -22.108  1.00 33.13      C
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ATOM    259  CE2 TYR B 106       7.234 -55.400 -23.569  1.00 32.27      C
ATOM    260  CZ  TYR B 106       7.219 -54.544 -22.487  1.00 33.19      C
ATOM    261  OH  TYR B 106       8.388 -54.291 -21.802  1.00 35.95      O
ATOM    262  N   VAL B 107       1.628 -54.270 -27.205  1.00 19.06      N
ATOM    263  CA  VAL B 107       0.557 -54.694 -28.099  1.00 18.06      C
ATOM    264  C   VAL B 107       1.015 -54.743 -29.559  1.00 17.45      C
ATOM    265  O   VAL B 107       0.502 -55.536 -30.346  1.00 16.99      O
ATOM    266  CB  VAL B 107      -0.690 -53.774 -27.978  1.00 20.95      C
ATOM    267  CG1 VAL B 107      -0.407 -52.407 -28.589  1.00 21.39      C
ATOM    268  CG2 VAL B 107      -1.879 -54.433 -28.658  1.00 21.30      C
ATOM    269  N   SER B 108       1.991 -53.916 -29.918  1.00 17.96      N
ATOM    270  CA  SER B 108       2.488 -53.892 -31.290  1.00 19.67      C
ATOM    271  C   SER B 108       3.197 -55.187 -31.694  1.00 20.38      C
ATOM    272  O   SER B 108       3.385 -55.449 -32.884  1.00 21.25      O
ATOM    273  CB  SER B 108       3.424 -52.691 -31.508  1.00 19.56      C
ATOM    274  OG  SER B 108       4.666 -52.824 -30.837  1.00 19.63      O
ATOM    275  N   GLY B 109       3.595 -55.995 -30.710  1.00 19.59      N
ATOM    276  CA  GLY B 109       4.251 -57.256 -31.023  1.00 20.03      C
ATOM    277  C   GLY B 109       3.311 -58.170 -31.792  1.00 19.61      C
ATOM    278  O   GLY B 109       3.579 -58.517 -32.940  1.00 19.24      O
ATOM    279  N   PRO B 110       2.206 -58.606 -31.173  1.00 19.20      N
ATOM    280  CA  PRO B 110       1.251 -59.478 -31.855  1.00 18.99      C
ATOM    281  C   PRO B 110       0.651 -58.761 -33.075  1.00 19.22      C
ATOM    282  O   PRO B 110       0.406 -59.371 -34.116  1.00 17.13      O
ATOM    283  CB  PRO B 110       0.198 -59.737 -30.778  1.00 20.41      C
ATOM    284  CG  PRO B 110       0.998 -59.720 -29.515  1.00 19.81      C
ATOM    285  CD  PRO B 110       1.914 -58.528 -29.729  1.00 19.94      C
ATOM    286  N   GLY B 111       0.407 -57.462 -32.927  1.00 19.03      N
ATOM    287  CA  GLY B 111      -0.160 -56.702 -34.025  1.00 19.60      C
ATOM    288  C   GLY B 111       0.764 -56.714 -35.226  1.00 19.59      C
ATOM    289  O   GLY B 111       0.330 -56.979 -36.339  1.00 21.10      O
ATOM    290  N   GLY B 112       2.043 -56.429 -34.995  1.00 19.78      N
ATOM    291  CA  GLY B 112       3.014 -56.417 -36.074  1.00 19.97      C
ATOM    292  C   GLY B 112       3.147 -57.783 -36.724  1.00 20.43      C
ATOM    293  O   GLY B 112       3.233 -57.896 -37.949  1.00 19.94      O
ATOM    294  N   LEU B 113       3.167 -58.828 -35.903  1.00 19.26      N
ATOM    295  CA  LEU B 113       3.265 -60.184 -36.429  1.00 19.49      C
ATOM    296  C   LEU B 113       2.040 -60.521 -37.274  1.00 18.73      C
ATOM    297  O   LEU B 113       2.143 -61.252 -38.255  1.00 18.44      O
ATOM    298  CB  LEU B 113       3.405 -61.198 -35.289  1.00 18.38      C
ATOM    299  CG  LEU B 113       4.777 -61.270 -34.605  1.00 20.59      C
ATOM    300  CD1 LEU B 113       4.656 -62.059 -33.311  1.00 20.01      C
ATOM    301  CD2 LEU B 113       5.794 -61.914 -35.538  1.00 20.23      C
ATOM    302  N   ALA B 114       0.875 -60.010 -36.892  1.00 18.96      N
ATOM    303  CA  ALA B 114      -0.334 -60.292 -37.661  1.00 18.70      C
ATOM    304  C   ALA B 114      -0.288 -59.578 -39.019  1.00 19.30      C
ATOM    305  O   ALA B 114      -0.602 -60.167 -40.052  1.00 20.62      O
ATOM    306  CB  ALA B 114      -1.562 -59.855 -36.889  1.00 16.45      C
ATOM    307  N   ALA B 115       0.082 -58.303 -39.000  1.00 20.57      N
ATOM    308  CA  ALA B 115       0.167 -57.516 -40.229  1.00 21.84      C
ATOM    309  C   ALA B 115       1.140 -58.192 -41.189  1.00 21.58      C
ATOM    310  O   ALA B 115       0.815 -58.464 -42.345  1.00 22.14      O
ATOM    311  CB  ALA B 115       0.636 -56.108 -39.911  1.00 19.85      C
ATOM    312  N   TRP B 116       2.334 -58.476 -40.688  1.00 22.12      N
ATOM    313  CA  TRP B 116       3.365 -59.126 -41.478  1.00 23.22      C
ATOM    314  C   TRP B 116       2.871 -60.434 -42.123  1.00 23.55      C
ATOM    315  O   TRP B 116       3.048 -60.643 -43.329  1.00 22.19      O
ATOM    316  CB  TRP B 116       4.584 -59.367 -40.579  1.00 26.08      C
ATOM    317  CG  TRP B 116       5.699 -60.136 -41.204  1.00 27.40      C
ATOM    318  CD1 TRP B 116       6.473 -59.761 -42.271  1.00 28.30      C
ATOM    319  CD2 TRP B 116       6.168 -61.418 -40.793  1.00 28.77      C
ATOM    320  NE1 TRP B 116       7.401 -60.742 -42.547  1.00 29.04      N
ATOM    321  CE2 TRP B 116       7.234 -61.771 -41.655  1.00 30.37      C
ATOM    322  CE3 TRP B 116       5.794 -62.308 -39.778  1.00 30.49      C
ATOM    323  CZ2 TRP B 116       7.929 -62.981 -41.529  1.00 31.08      C
ATOM    324  CZ3 TRP B 116       6.485 -63.510 -39.653  1.00 31.85      C
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ATOM    325  CH2 TRP B 116       7.541 -63.834 -40.527  1.00 32.27      C
ATOM    326  N   SER B 117       2.231 -61.304 -41.338  1.00 21.35      N
ATOM    327  CA  SER B 117       1.735 -62.573 -41.873  1.00 22.61      C
ATOM    328  C   SER B 117       0.665 -62.383 -42.940  1.00 23.56      C
ATOM    329  O   SER B 117       0.463 -63.262 -43.780  1.00 23.11      O
ATOM    330  CB  SER B 117       1.167 -63.462 -40.756  1.00 20.72      C
ATOM    331  OG  SER B 117       0.010 -62.889 -40.169  1.00 22.72      O
ATOM    332  N   LEU B 133      11.788 -52.846 -25.860  1.00 23.38      N
ATOM    333  CA  LEU B 133      11.903 -54.293 -26.020  1.00 24.54      C
ATOM    334  C   LEU B 133      11.209 -54.833 -27.276  1.00 22.84      C
ATOM    335  O   LEU B 133      11.784 -55.619 -28.027  1.00 21.86      O
ATOM    336  CB  LEU B 133      11.328 -54.996 -24.786  1.00 25.48      C
ATOM    337  CG  LEU B 133      11.388 -56.527 -24.780  1.00 27.50      C
ATOM    338  CD1 LEU B 133      12.840 -56.984 -24.866  1.00 28.69      C
ATOM    339  CD2 LEU B 133      10.735 -57.059 -23.509  1.00 28.04      C
ATOM    340  N   THR B 134       9.975 -54.401 -27.499  1.00 21.72      N
ATOM    341  CA  THR B 134       9.202 -54.860 -28.639  1.00 21.22      C
ATOM    342  C   THR B 134       9.693 -54.326 -29.986  1.00 20.62      C
ATOM    343  O   THR B 134       9.843 -55.091 -30.932  1.00 20.33      O
ATOM    344  CB  THR B 134       7.716 -54.509 -28.449  1.00 20.99      C
ATOM    345  OG1 THR B 134       7.257 -55.075 -27.210  1.00 20.94      O
ATOM    346  CG2 THR B 134       6.872 -55.073 -29.600  1.00 20.64      C
ATOM   3608  N   LYS B 136      12.595 -53.366 -30.809  1.00 21.46      N
ATOM   3609  CA  LYS B 136      13.886 -53.949 -31.144  1.00 22.79      C
ATOM   3610  CB  LYS B 136      14.713 -54.196 -29.879  1.00 24.70      C
ATOM   3611  CG  LYS B 136      16.183 -54.424 -30.178  1.00 27.75      C
ATOM   3612  CD  LYS B 136      16.998 -54.494 -28.902  1.00 30.17      C
ATOM   3613  CE  LYS B 136      18.479 -54.671 -29.203  1.00 32.33      C
ATOM   3614  NZ  LYS B 136      19.278 -54.641 -27.944  1.00 33.37      N
ATOM   3615  C   LYS B 136      13.793 -55.229 -31.966  1.00 23.46      C
ATOM   3616  O   LYS B 136      14.561 -55.407 -32.912  1.00 23.71      O
ATOM    347  N   TRP B 137      12.868 -56.127 -31.633  1.00 21.78      N
ATOM    348  CA  TRP B 137      12.753 -57.345 -32.424  1.00 22.06      C
ATOM    349  C   TRP B 137      11.768 -57.202 -33.574  1.00 21.75      C
ATOM    350  O   TRP B 137      11.936 -57.822 -34.623  1.00 21.76      O
ATOM    351  CB  TRP B 137      12.361 -58.552 -31.553  1.00 21.20      C
ATOM    352  CG  TRP B 137      10.990 -58.525 -30.922  1.00 20.23      C
ATOM    353  CD1 TRP B 137      10.696 -58.231 -29.618  1.00 19.62      C
ATOM    354  CD2 TRP B 137       9.748 -58.877 -31.544  1.00 18.68      C
ATOM    355  NE1 TRP B 137       9.349 -58.385 -29.390  1.00 19.31      N
ATOM    356  CE2 TRP B 137       8.743 -58.780 -30.555  1.00 18.97      C
ATOM    357  CE3 TRP B 137       9.383 -59.270 -32.840  1.00 19.75      C
ATOM    358  CZ2 TRP B 137       7.401 -59.058 -30.821  1.00 18.18      C
ATOM    359  CZ3 TRP B 137       8.046 -59.549 -33.107  1.00 18.87      C
ATOM    360  CH2 TRP B 137       7.072 -59.440 -32.099  1.00 18.94      C
ATOM    361  N   LEU B 138      10.741 -56.381 -33.386  1.00 21.61      N
ATOM    362  CA  LEU B 138       9.744 -56.188 -34.431  1.00 23.15      C
ATOM    363  C   LEU B 138      10.384 -55.558 -35.676  1.00 23.07      C
ATOM    364  O   LEU B 138       9.958 -55.801 -36.809  1.00 22.68      O
ATOM    365  CB  LEU B 138       8.618 -55.305 -33.886  1.00 23.87      C
ATOM    366  CG  LEU B 138       7.312 -55.155 -34.664  1.00 26.48      C
ATOM    367  CD1 LEU B 138       6.672 -56.508 -34.915  1.00 25.34      C
ATOM    368  CD2 LEU B 138       6.383 -54.267 -33.851  1.00 25.90      C
ATOM   3644  N   LYS B 140      12.801 -56.332 -37.241  1.00 27.38      N
ATOM   3645  CA  LYS B 140      13.279 -57.337 -38.182  1.00 28.05      C
ATOM   3646  CB  LYS B 140      13.893 -58.501 -37.401  1.00 29.91      C
ATOM   3647  CG  LYS B 140      15.134 -58.057 -36.635  1.00 31.62      C
ATOM   3648  CD  LYS B 140      15.719 -59.149 -35.757  1.00 33.53      C
ATOM   3649  CE  LYS B 140      16.974 -58.634 -35.055  1.00 34.46      C
ATOM   3650  NZ  LYS B 140      17.692 -59.713 -34.320  1.00 36.17      N
ATOM   3651  C   LYS B 140      12.254 -57.833 -39.212  1.00 27.83      C
ATOM   3652  O   LYS B 140      12.602 -58.562 -40.142  1.00 27.80      O
ATOM    369  N   ILE B 141      10.992 -57.445 -39.052  1.00 26.40      N
ATOM    370  CA  ILE B 141       9.963 -57.818 -40.016  1.00 26.09      C
ATOM    371  C   ILE B 141       9.316 -56.542 -40.530  1.00 25.81      C
ATOM    372  O   ILE B 141       8.353 -56.586 -41.305  1.00 26.10      O
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ATOM	373	CB	ILE	B	141	8.854	-58.721	-39.405	1.00	26.39	C
ATOM	374	CG1	ILE	B	141	8.298	-58.09-23-	-38.127	1.00	26.45	C
ATOM	375	CG2	ILE	B	141	9.401	-60.118	-39.145	1.00	28.33	C
ATOM	376	CD1	ILE	B	141	7.136	-58.845	-37.549	1~00	26.95	C
TER											

The following examples are presented for purposes of illustration only and are not intended to limit the scope of the invention in any way.

EXAMPLE I

This example describes the crystallization of the *E. coli* MurG protein and the determination of the coordinates of the three-dimensional crystal structure. This example also describes the identification of the donor nucleotide binding site, the acceptor binding site and the membrane association site of the MurG protein.

Abstract

The 1.9 Å X-ray structure of a membrane-associated glycosyltransferase involved in peptidoglycan biosynthesis is reported. This enzyme, MurG, contains two α/β open sheet domains separated by a deep cleft. The C-terminal domain contains the LTDP-GlcNAc binding site while the N-terminal domain contains the acceptor binding site and likely membrane association site. Combined with sequence data from other MurG homologs, this structure provides insight into the residues that are important in substrate binding and catalysis. We have also noted that a conserved region *found in* many UDP-sugar transferases maps to a $\beta/\alpha/\beta/\alpha$ supersecondary structural motif in the donor binding region of MurG, an observation that is be helpful in glycosyltransferase structure prediction.

Methods

Crystallization

E. coli MurG containing a C-terminal LEHHHHHH sequence was purified as described(Ha et al., 1999) and concentrated to 10 mg ml-' in 20 mM Tris-HCI, pH 7.9/ 150 mM NaCl/ 50 mM EDTA. The protein concentrate was mixed with UDP-GlcNAc in a 1:3 molar ratio. Crystals were grown at room temperature using the hanging-drop vapor-diffusion method by mixing equal volumes of protein with reservoir solution (0. 1 M NaMES, pH 6.5/ 0.96 M (NH,),SO,/ 0.4% Triton X-100/

10 mM DTT). Triclinic crystals with a typical size of 0.2 mm X 0.1 mm X 0.1 mm grew within a week. The crystals belong to the PI space group, with two molecules per asymmetric unit. The cell dimensions are a=60.613 Å, b=66.356 Å, c=67.902 Å, α =64.294, β =83.520, γ =65.448

Data collection and processing

All data sets were collected at 100 K on previously flash frozen crystals. Crystals were equilibrated in a cryoprotectant buffer with 0.1 M NaMES, pH 6.5, 1.44 M $(NH_4)_2SO_4$, 0.4% Triton X-100, and 20% glycerol. Heavy-atom soaks were carried out in the same buffer containing one of the following heavy-atom solutions: 2 mM $HgCl_2$, 1 mM $(NH_4)_2WS_4$, 1 mM $(NH_4)_2OsBr_6$. Crystals were flash-frozen in liquid nitrogen. HgC_2 (form A derivative) and $(NH_4)_2OsBr_6$ derivative data were collected at an R-AXISIIC imaging plate detector mounted on a Rigaku 200HB generator. Native, $HgCl_2$ (form B derivative), and $(NH_4)_2WS_4$ derivative diffraction data were collected at beam-line BioCARS-14B at the Advanced Photon Source, at wavelengths 1.0092 Å, 0.9900 Å and 1.2147 Å respectively. Collection of data on the $HgCl_2$, derivative was initially designed for MAD phasing; however, the mercury derivative proved to be unstable to X-rays, and after a two-hour exposure to synchrotron radiation the form A derivative metamorphosed into a different mercury derivative (form B) that was suitable for MIR phasing. All the data were reduced using DENZO and SCALEPACK (Otwinowski & Minor, 1997), and processed with CCP4 programs (CCP4, 1994).

Structure determination and refinement

The structure was solved by multiple isomorphous replacement combined with anomalous scattering of mercuric derivatives (Table 1). Initial MIR phases calculated with program MLPHARE had a mean figure of merit of 0.44 to 2.5 Å, and were improved by solvent flattening and histogram matching using DM. An MIR map was generated which had continuous electron density for most regions of the protein. A model was built with the program O (Jones et al., 1991), and the structure was refined against 1.9 Å data using energy minimization, simulated annealing and B-factor refinement with the program CNS (Brunger et at., 1998). The N-terminal six residues and the C-terminal His-tag had no electron density and were not included in this model. There was no electron density for UDP-GlcNAc.

Results and discussion

Overall fold

The crystal structure of E. coli MurG was solved by a combination of multiple isomorphous replacement and anomalous scattering, and refined to 1.9 Å resolution (Table 1).

TABLE 1

Summary of crystallographic and refinement data

Data set	Native	$HgCl_2$ (form A derivative)	$HgCl_2$ (form B derivative)	$(NH_4)_2WS_4$	$(NH_4)_2OsBr_6$
Resolution (Å)	1.9	2.0	1.9	2.4	2.3
Observations	288,150	101,913	245,320	44,366	106,606
Unique reflections	65,567	53,391	65,581	27,950	36,443
R_{sym}[1] (last shell)	0.032 (0.187)	0.043 (0.200)	0.042 (0.296)	0.031 (0.080)	0.056 (0.302)
I/σ (last shell)	41.9(7.0)	20.4(2.9)	29.0(3.7)	24.6(8.2)	19.6(2.5)
Completeness (last shell)	97.7% (96.4%)	91.4% (66.6%)	97.4% (94.0%)	83.8% (62.0%)	94.3% (78.6%)
MIR analysis (40.0 - 2.5 Å)					
Mean isomorphous difference[2]		0.163	0.130	0.068	0.134
Phasing power[3] (last shell)		1.09(0.73)	0.57(0.50)	0.61(0.24)	0.61(0.58)
R_{cullis}[4](last shell)		0.81 (0.91)	0.94(0.96)	0.92(0.99)	0.94(0.95)
Anomalous R_{cullis}[4](last shell)		0.96(1.00)	0.95(1.00)		

Refinement statistics			
Resolution	40.0 - 1.9 Å	R. m. s. d.[7]	
Reflections ($\|F\| > 2\sigma$)	61,989	Bonds (Å)	0.006
Protein atoms (a. u.)	5,280	Angles(°)	1.29
Water Atoms	298		
Sulfate groups	1	Ramachandran plot[8]	
R-factor-[5]	22.0%	Residues in most favored region	94.6%
R-free[6]	24.7%	Residues in additional allowed region	5.4%

[1] $R_{sym} = \Sigma| I_i - \langle I \rangle | / \Sigma I_i$, where I_i is the intensity of a reflection, and $\langle I \rangle$ is the average intensity of that reflection.
[2] Mean isomorphous difference = $\Sigma |F_{PH}-F_P|/\Sigma F_{PH}$, where F_{PH} and F_P are the derivative and native structure factors respectively.
[3] Phasing power is the ratio of the mean calculated derivative structure factor to the mean lack of closure error.
[4] R_{cullis} is the mean residual lack of closure error divided by the dispersive or anomalous difference.
[5] R-factor = $\Sigma|Fobs| - |Fcalc| | /\Sigma| F|$
[6] R-free is the R-factor calculated using 10% of the reflection data chosen randomly and omitted from the start of refinement.
[7] R. m. s. d., root-mean-square deviations from ideal bond lengths and bond angles.
[8] Calculated with program PROCHECK.

The structure consists of two domains separated by a deep cleft (Fig. 2a). Both domains exhibit an α/β open-sheet structure and have high structural homology despite minimal sequence homology (RMSD = 2.02 over 85 aligned Cα atoms). The N-domain includes residues 7-163 and 341-357, and contains seven parallel β-strands and six α -helices, the last of which originates in the C-domain (Fig. 2b). The C-domain comprises residues 164-340 and contains six parallel β-strands and eight α -helices, including one irregular bipartite helix (α-link) that connects the N-domain to the first β-strand of the C-domain. The β-strands in both domains are ordered as for a typical Rossman fold. The N- and C-domains are joined by a short linker between the seventh β-strand of the N-domain and the α-link of the C-domain. This inter-domain linker and the peptide segment that joins the last helix of the C-domain to the last helix of the N-domain define the floor of the cleft between the two domains. The cleft itself is about 20 Å deep and 18 Å across at its widest point. Contacts < 4 Å across the cleft are limited primarily to interactions between residues from C-α5 to the loop connecting N-β5 to N-α5.

The α/β open-sheet motif (Rossman fold) adopted by both the N- and C-domains of MurG is characteristic of domains that bind nucleotides (Branden & Tooze, 1998). Classical Rossman domains typically contain at least one conserved glycine rich motif, with the consensus sequence GXGXXG, located at a turn between the carboxyl end of one β-strand and the amino terminus of the adjacent α-helix (Baker et al., 1992). This motif is involved in binding the negatively charged phosphates (Carugo & Argos, 1997). There are three glycine rich loops (G loops) in *E. coli* MurG (Fig. 3a) that may be variants on the phosphate binding loops found in other dinucleotide binding proteins (see below).

Sequence homology

Amino acid sequences for eighteen MurG homologs are now available. The sequence similarity between *E. coli* MurG and homologs from other bacterial strains ranges from less than 30% to more than 90% depending on the evolutionary relationship between the organisms. In all MurG homologs, however, there are several invariant residues. Fig. 3a shows a sequence alignment for a subset of MurG homologs with the invariant and highly conserved residues indicated. These residues,

which include the three G loops, have been highlighted in the *E. coli* MurG structure (Fig. 3b). Almost all of the invariant residues are located at or near the cleft between the two domains. Two of the G loops are found in the N domain (between N-β1/N-αl and N-β4/N-α4) and one is found in the C-domain (between C-β1/C-αl). The strict conservation of the highlighted residues among different bacterial strains, and their location as determined from the *E. coli* MurG structure, implicates them in substrate binding and catalytic activity.

Structural homology reveals the donor binding site

The three-dimensional backbone structure of *E. coli* MurG was compared to known protein structures, including the three other NDP-glycosyltransferase structures that have been reported (Chamok & Davies, 1999; Gastinel *et al.,* 1999; Vrielink *et al.,* 1994). The C-terminal domain was found to have significant structural homology (RMSD= 2.218 Å for 89 aligned C? atoms) to the C-terminal domain of phage T4 β-glucosyltransferase (BGT), an enzyme that catalyzes the glucosylation of hydroxymethyl-cytosines in duplex DNA. A co-crystal structure of BGT with UDP bound in the C-terminal domain reveals the topology of the UDP binding pocket and also shows important contacts to the nucleotide (Moréra *et al.,* 1999; Vrielink *et al.,* 1994). These contacts include: a) hydrogen bonds from the backbone amide of 1238 to the N3 and O4 positions of the base; b) hydrogen bonds between the carboxyl side chain of E272 and the O2' and O3' hydroxyls of the ribose ring; and c) contacts from a GGS motif in the loop following the first β-strand of the C domain to the alpha phosphate of UDP. The structurally homologous C-domain of MurG contains a topologically similar pocket (Fig. 4a). Furthermore, even though the two domains share only 11% sequence identity overall, there are identical residues in the same spatial location in *E. coli* MurG and in BGT. Based on this comparison, we have concluded that the C-domain of *E. coli* MurG is the UDP-GlcNAc binding site.

We have docked UDP-GlcNAc into the C-domain of E. coli MurG using the information on how UDP binds to BGT as a guide. As shown in Figure 4b, the uracil is held in place by contacts from the N3 and O4 atoms to the backbone amide of I245. The O2' and O3' hydroxyls on the ribose sugar are within hydrogen bonding distance of the invariant glutamate residue (E269) in the middle of helix C-?4. The conserved GGS motif in G loop 3 is positioned to contact the alpha phosphate. When these

contacts are made, the UDP-GlcNAc substrate fits nicely into a pocket in the C-domain, where it is surrounded by many of the invariant residues identified through sequence analysis of other MurG homologs. It is possible to propose roles for some of these invariant residues from the model. For example, the side chain of R261 can be rotated to contact the second phosphate; this contact may help explain why UDP binds significantly better to MurG than UMP. We propose that R261 plays an important role in catalysis by stabilizing the UDP leaving group via electrostatic interactions. The side chain of Q289 is within hydrogen bonding distance of the C4 hydroxyl of the GlcNAc sugar. This contact may explain why MurG can discriminate between UDP-GlcNAc and its C4 axial isomer, UDP-GalNAc (Ha *et at.,* 1999).

The acceptor binding site

Structural considerations suggest that the primary acceptor binding site is located in the N-terminal domain of MurG. This domain contains three highly conserved regions, two of which are glycine-rich loops that face the cleft (Fig 3a and 4c). These G loops are reminiscent of the phosphate binding loops found in other nucleotide binding proteins, and are most likely involved in binding to the diphosphate on Lipid I. The N-termini of the helices following each G loop form opposite walls of a small pocket between the G loops. The helix dipoles create a positively charged electrostatic field in the pocket that can stabilize the negative charged diphosphates. When the diphosphate of the acceptor is anchored in the pocket created by the G-loops, the MurNAc sugar emerges into the cleft between domains and the C4 hydroxyl can be directed towards the anomeric carbon of the GlcNAc for attack on the face opposite the UDP leaving group. The third conserved region in the N domain spans the loop from the end of N-?5 to the middle of N-?5. Kinetic analysis of mutants is required to evaluate the roles of these residues (Ha *et al.,* 1999; Men *et al.,* 1998).

Proposed membrane association site

MurG associates with the cytoplasmic surface of bacterial membranes where it couples a soluble donor sugar to the membrane anchored acceptor sugar, Lipid I. Analysis of the *E. coli* MurG structure shows that there is a hydrophobic patch consisting of residues I75, L79, F82, W85 and W116 in the N-domain, which is surrounded by basic residues (K72, K140, K69, R80, R86, R89). We propose that this

is the membrane association site and that association involves both hydrophobic and electrostatic interactions with the negatively charged bacterial membrane. The location of this patch in MurG is also consistent with the proposed acceptor binding site: membrane association at this patch would bring the two N-terminal G loops close to the membrane surface where the diphosphate portion of the acceptor is located (Fig. 4c). Moreover, the cleft between the two domains would remain accessible, consistent with the biochemical requirement that the soluble UDP-GlcNAc donor be able to find its binding site from the cytoplasm.

Implications for other glycosyltransferases

Glycosyltransferases that utilize an activated nucleotide sugar as a donor comprise a large family of enzymes in both prokaryotes and eukaryotes, and they play central roles in many important biological processes (Dennis *et al.*, 1999; Koya *et al.*, 1999; Verbert & Cacan, 1999). Glycosyltransferases are typically classified according to the nucleotide sugar they utilize, and it has frequently been noted that there is no significant sequence homology even among glycosyltransferases in the same family. This has made it difficult to identify common structural features and residues important in binding and catalysis. There are only three other glycosyltransferase structures available, and although none of them shows any sequence homology to MurG, a structural comparison indicates that one of them, BGT, contains a related donor binding site.

In addition to this structural homology, we have identified a strikingly similar sequence motif in the MurG family and certain other UDP-glycosyltransferase families. This sequence motif spans about a thirty amino acid stretch in the C-domain of MurG and includes most of the invariant residues found in that domain. As shown in Figure 3a, a similar motif is found in the UDP-glucuronosyltransferases (Mackenzie, 1990). Certain residues are identical, including a number of prolines and glycines, and the spacing between them is invariant. This suggests that the UDP-glucuronosyltransferases contain a region of α/β supersecondary structure that is involved in a similar function as the corresponding region in MurG (Fig. 3c). This region binds the donor sugar. By analyzing the similarities and differences between the conserved residues in this subdomain in the MurG family and other UDP-glycosyltransferase families, it may be possible to identify - and perhaps alter - residues that are involved in determining donor

selectivity. We note that it would be useful to be able to manipulate donor specificity because it would extend the utility of glycosyltransferases as reagents for glycosylation of complex molecules. Altered glycosyltransferases could also be useful for remodeling cell surfaces and for probing the biological roles of particular carbohydrate structures.

Conclusion

This first structure of a member of the MurG family of glycosyltransferases lays the groundwork for further mechanistic and structural investigations, which may lead to the design of inhibitors and perhaps even new antibiotics. The work also shows that there can be conserved subdomains even in very different glycosyltransferase families. Information on conserved subdomains will be useful for structure prediction and may help guide experiments directed towards changing substrate specificity.

EXAMPLE2

This example describes a method of isolating the C-terminal domain of the *E. coli* MurG protein, expressing the domain in *E. coli* cells and utilizing nuclear magnetic resonance (NMR) to determine the ability of compounds to bind.

MurG can also be used to determine the ability of a chemical compound to bind to the C domain by a) determining the start of c domain based on the MurG crystal structure; b) independently expressing the C domain; and c) using NMR methods to identify binding site and/or bound conformation of ligand. The same procedure is used for the acceptor binding domains.

NMR methods are used to identify the protein binding sites and screen for ligands that bind. The MurG C-terminal domain region of the protein has been expressed independently. The C domain has a much lower molecular weight than the full-length protein. Therefore, the expression of the C domain results in much sharper NMR peaks which will facilitate the NMR interpretation. Also the proton chemical shifts are very sensitive to their environment. Binding of a compound will introduce local environment changes, thus changing the proton chemical shifts. In this way, residues involved in the binding can be differentiated easily from other amino acid residues not involved in binding a ligand. This method has also been used to identify ligands that bind to low molecular weight drug targets (i.e., small proteins).

Relevant references to NMR techniques are: Discovering high-affinity ligands for proteins: SAR by NMR, S. Shuker, P. Hajduk, R. Meadows, and S. Fesik, Science 274, 1531 (1996); Lin Y, Nageswara Rao BD. Structural characterization of adenine nucleotides bound to Escherichia coli adenylate kinase. 1. Adenosineconformations by proton two-dimensional transferred nuclear Overhauser effect spectroscopy. Biochemistry. 2000 Apr 4;39(13):3636-46; and Fejzo J, et al., Chem Biol 1999 Oct,6(10):755-69 (incorporated herein by reference).

The SHAPES strategy is also useful for NMR identification of binding residues, ligands and drug discover which is an NMR-based approach for lead generation in drug discovery. Recently, it has been shown that nuclear magnetic resonance (NMR) may be used to identify ligands that bind to low molecular weight protein drugtargets. Recognizing the utility of NMR as a very sensitive method for detecting binding, we have focused on developing alternative approaches that are applicable to larger molecular weight drug targets and do not require isotopic labeling. A new method for lead generation (SHAPES) uses NMR to detect the binding of a limited but diverse library of small molecules to a potential drug target. The compound scaffolds are derived from shapes most commonly found in known therapeutic agents. NMR detection of low (microM-mM) affinity binding is achieved using either differential line broadening or transferred NOE (nuclear Overhauser effect) NMR techniques. The SHAPES method for lead generation by NMR is useful for identifying potential lead classes of drugs early in a drug design program, and is easily integrated with other discovery tools such as virtual screening, high-throughput screening and combinatorial chemistry.

EXAMPLE 3

This example describes the method of using the three-dimensional structure of *E. coli* MurG to determine the crystal structures of its mutant, enzyme-ligand complex, and MurG homologs, which share the same folding motif.

First, a crystalline form of the new protein or the protein complex should be obtained. The E.coli MurG mutants should be crystallized in a condition very similar to what we have showed in the method section. The.protein-ligand complex can be obtained by soaking the protein crystals in a ligand-containing buffer. Other MurG homologs can be expressed in a His-tagged fashion and purified using affinity colume.

Presumably they can be crystallized in a similar way using a detergent as the additive. Next, the diffraction data should be collected and processed. After the data collection, the molecular replacement method is used to determine the unknown structure. Either the whole *E. coli* MurG protein or one single domain can serve as a search model. This search model can be rotated and translated until the correct orientation is located in the unit cell of this unknown structure. The search model may only represent part of the contents of the asymmetric unit. However, the location of the first model is now already available. While the first location of the search model is fixed, the second round of translation search can be carried out to search more molecules or domains in the asymmetric unit cell. The phases from the final model generated by molecular replacement can be used to calculate the electron density map. Finally, a model is built based on the electron density map, and the model needs to be refined using program CNS or XPLOR.

EXAMPLE 4

This example describes the method of using the three-dimensional coordinate structure of *E. coli* MurG to produce a protein fragment that can be used in an NMR-based lead discovery program. The crystal structure reveals the boundaries of the C domain and permits us to design a gene containing only the C domain from the gene containing both domains. The C domain starting at residue 164 and ending at residue 340 was cloned into an expression vector to generate a C-terminal His-tag fusion, It was over-expressed in *E. coli* cells and purified by affinity colume. The protein was shown to be monomeric by size exclusion chromatography and to be soluble at least up to 0.15 mM, a concentration more than adequate for NMR analysis. C domains from other MurG homologues can be similarly expressed and used.

EXAMPLE 5

This example describes the co-crystallization of a MurG protein with a ligand. A MurG-ligand complex is formed by either co-crystallizing MurG protein with appropriate ligand or soaking the MurG crystals in buffers containing appropriate ligand. Co-crystallization is done by pre-mixing the protein sample with a certain amount of substrate or substrate analogs. Then the hanging drop method is used to produce crystals as described infra.

Alternatively, ligans are incorporated into the crystals by soaking the protein crystals in the ligand containing buffer for a period of time to allow for infiltration into the crystal. The time ranges from a couple of hours to a couple of days. The concentration of ligand in the buffer ranges from several milimolar to several hundred mili molar.

DEPOSIT OF COORDINATES

The crystal structure three-dimensional coordinates of the *E. coli* MurG as set forth in Table 1 were deposited with the Protein Data Bank and have been assigned the indicated ID Code (Accession No.) 1F0K.

Although the invention is described in detail with reference to specific embodiments thereof, it will be understood that variations which are functionally equivalent are within the scope of this invention. Indeed, various modifications of the invention in addition to those shown and described herein will become apparent to those skilled in the art from the foregoing description and accompanying drawings. Such modifications are intended to fall within the scope of the appended claims.

Various publications are cited herein, the disclosures of which are incorporated by reference in their entireties.

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WHAT IS CLAIMED IS:

1. A composition comprising the *E. coli* MurG protein in crystalline form.

2. A composition comprising a MurG protein in crystalline form.

3. A three-dimensional structure of the crystalline form of an *E. coli* MurG protein, wherein the three-dimensional structure substantially conforms to the atomic coordinates represented in Table 1.

4. A three-dimensional structure of the crystalline form of a MurG protein, wherein the three-dimensional structure substantially conforms to the atomic coordinates represented in Table 1.

5. A three-dimensional structure of the α-carbon backbone of the crystalline form of an *E. coli* MurG protein, wherein the three-dimensional structure substantially conforms to the atomic coordinates represented in Table 2.

6. A three-dimensional structure of the α-carbon backbone and conserved amino acid residues of an E coli MurG protein, wherein the three-dimensional structure substantially conforms to the atomic coordinates represented in Table 3.

7. A three-dimensional structure of a donor nucleotide binding site of a MurG protein wherein the three-dimensional structure structure of the donor nucleotide binding site substantially conforms to the atomic coordinates in Table 4.

8. The three-dimensional structure of claim 7, wherein the donor nucleotide is UDP-GlcNAc.

9. A three-dimensional structure of an acceptor binding site of a MurG protein substantially conforming to the atomic coordinates in Table 5.

10. A three-dimensional structure of a membrane association site of a MurG protein substantially conforming to the atomic coordinates in Table 6.

11. A three-dimensional computer image of the three-dimensional structure of a MurG protein.

12. The image of claim 11, wherein the structure substantially conforms with the three-dimensional coordinates listed in Table 1.

13. The image of claim 11, wherein the computer image that is generated when a set of three-dimensional coordinates comprising the three-dimensional coordinates represented in Table 1 are analyzed on a computer using a graphical display software program to create an electronic file of the image and visualizing the electronic

file on a computer capable of representing the electronic file as a three-dimensional image.

14. The image of claim 11, wherein the three-dimensional computer image is represented by a two dimensional image selected from the group consisting of Fig. 2a, 3a, or 4c.

15. The image of claim 11, wherein the three-dimensional computer image is used to design a compound.

16. A three-dimensional computer image of the three-dimensional structure of the α-carbon backbone of a MurG protein.

17. The image of claim 16, wherein the structure substantially conforms with the three-dimensional coordinates listed in Table 2.

18. The image of claim 16, wherein the computer image is that is generated when a set of three-dimensional coordinates comprising the three-dimensional coordinates represented in Table 2 are analyzed on a computer using a graphical display software program to create an electronic file of the image and visualizing the electronic file on a computer capable of representing the electronic file as a three-dimensional image.

19. The image of claim 16, wherein the three-dimensional computer image is used to design a compound.

20. A three-dimensional image of the three-dimensional image of an α-carbon backbone and conserved amino acid residues of a MurG protein.

21. The image of claim 20, wherein the structure substantially conforms with the three-dimensional coordinates in Table 3.

22. The image of claim 21, wherein the computer image is that is generated when a set of three-dimensional coordinates comprising the three-dimensional coordinates represented in Table 3 are analyzed on a computer using a graphical display software program to create an electronic file of the image and visualizing the electronic file on a computer capable of representing the electronic file as a three-dimensional imaie.

23. The image of claim 21, wherein the three-dimensional computer image is used to design a compound.

24. A three-dimensional computer image of the three-dimensional structure of a donor nucleotide binding site of a MurG protein.

25. The image of claim 24, wherein the structure substantially conforms with the three-dimensional coordinates in Table 4.

26. The image of claim 24, wherein the computer image is that is generated when a set of three-dimensional coordinates comprising the three-dimensional coordinates represented in Table 4 are analyzed on a computer using a graphical display software program to create an electronic file of the image and visualizing the electronic file on a computer capable of representing the electronic file as a three-dimensional image.

27. The image of claim 24, wherein the three-dimensional computer image is rep resented by a two dimensional image selected from the group consisting of Fig. 3c, 4a or 4b.

28. The image of claim 24, wherein the three-dimensional computer image is used to design a compound.

29. A three-dimensional computer image of the three-dimensional structure of an acceptor binding site of a MurG protein.

30. The image of claim 29, wherein the structure substantially conforms with the three-dimensional coordinates Table 5.

31. The image of claim 29, wherein the computer image is that is generated when a set of three-dimensional coordinates comprising the three-dimensional coordinates represented in Table 5 are analyzed on a computer using a graphical display software program to create an electronic file of the image and visualizing the electronic file on a computer capable of representing the electronic file as a three-dimensional image.

32. The image of claim 29, wherein the three-dimensional computer image is represented by the two dimensional image of Fig. 4a.

33. The image of claim 29, wherein the three-dimensional computer image is used to design a compound.

34. A three-dimensional computer image of the three-dimensional structure of a membrane association site of a MurG protein.

35. The image of claim 34, wherein the structure substantially conforms with the three-dimensional coordinates Table 6.

36. The image of claim 34, wherein the computer image is that is generated when a set of three-dimensional coordinates comprising the three-dimensional coordinates represented in Table 6 are analyzed on a computer using a graphical display software program to create an electronic file of the image and visualizing the electronic file on a computer capable of representing the electronic file as a three-dimensional image.

37. The image of claim 34, wherein, the three-dimensional computer image is represented by the two dimensional image of Fig. 4a.

38. The image of claim 34, wherein the three-dimensional computer image is used to design a compound.

39. A computer readable medium encoded with a set of three-dimensional coordinates of a MurG protein having a three-dimensional structure that substantially conforms to the atomic coordinates of Table 1, wherein using a graphical display software program, the three-dimensional coordinates create an electronic file that can be visualized on a computer capable of representing said electronic file as a three-dimensional image.

40. A computer readable medium encoded with a set of three-dimensional coordinates of an α-carbon backbone of a MurG protein having a three-dimensional structure that substantially conforms to the atomic coordinates of Table 2, wherein using a graphical display software program, the three-dimensional coordinates create an electronic file that can be visualized on a computer capable of representing said electronic file as a three-dimensional image.

41. A computer readable medium encoded with a set of three-dimensional coordinates of an α-carbon backbone and conserved amino acid residues of a MurG protein having a three-dimensional structure that substantially conforms to the atomic coordinates of Table 3, wherein using a graphical display software program, the three-dimensional coordinates create an electronic file that can be visualized on a computer capable of representing said electronic file as a three-dimensional image.

42. A computer readable medium encoded with a set of three-dimensional coordinates of a donor nucleotide binding site of a MurG protein having a three-

dimensional structure that substantially conforms to the atomic coordinates of Table 4, wherein using a graphical display software program, the three-dimensional coordinates create an electronic file that can be visualized on a computer capable of representing said electronic file as a three-dimensional image.

43. A computer readable medium encoded with a set of three-dimensional coordinates of an acceptor binding site of a MurG protein having a three-dimensional structure that substantially conforms to the atomic coordinates of Table 5, wherein using a graphical display software program, the three-dimensional coordinates create an electronic file that can be visualized on a computer capable of representing said electronic file as a three-dimensional image.

44. A computer readable medium encoded with a set of three-dimensional coordinates of a membrane association site of a MurG protein having a three-dimensional structure that substantially conforms to the atomic coordinates of Table 5, wherein using a graphical display software program, the three-dimensional coordinates create an electronic file that can be visualized on a computer capable of representing said electronic file as a three-dimensional image.

45. A method for identifying a potential inhibitor of a UDP-glycosyltransferase enzyme, the method comprising the steps of:

(a) using a three-dimensional structure of UDP-glycosyltransferase enzyme as defined by atomic coordinates of UDP-glycosyltransferase enzyme according to FIG. 5;

(b) employing said three-dimensional structure to design or select said potential inhibitor;

(c) synthesizing said potential inhibitor; and

(d) contacting said potential inhibitor with said UDP-glycosyltransferase enzyme in the presence of a substrate to test the ability of said potential inhibitor to inhibit said UDPglycosyltransferase enzyme.

46. The method according to claim 45, wherein said potential inhibitor is selected from a database.

47. The method according to claim 45, wherein said potential inhibitor is designed de novo.

48. The method according to claim 45, wherein said potential inhibitor is designed from a known inhibitor.

49. The method according to claim 45, wherein said step of employing said three-dimensional structure to design or select said potential inhibitor comprises the steps of:

(a) identifying chemical entities or fragments capable of associating with UDP-glycosyltransferase enzyme; and

(b) assembling the identified chemical entities or fragments into a single molecule to provide the structure of said potential inhibitor.

50. The method according to claim 45, wherein the potential inhibitor is a competitive inhibitor of mutant UDP-glycosyltransferase enzyme.

51. The method according to claim 45, wherein said potential inhibitor is a noncompetitive or uncompetitive inhibitor of mutant UDP-glycosyltransferase enzyme.

52. A model of a UDP-glycosyltransferase, wherein the model represents a three-dimensional structure that substantially conforms to the atomic coordinates of Table 1.

53. The model of claim 52, wherein the structure substantially conforms to the atomic coordinates and B-values represented by Table 1.

54. The model of claim 52, wherein the structure is monomeric.

55. The model of claim 52, wherein at least about 50% of the structure has an average root-mean-square deviation (RMDS) of less than about 2.5 Å for backbone atoms in secondary structure elements in each domain of the structure.

56. The model of claim 52, wherein the MurG protein comprises an amino acid sequence that is at least about 25% identical to the amino acid sequence of the *E. coli* MurG protein.

57. The model of claim 52, wherein the MurG protein comprises an amino acid sequence that is at least about 40% identical to the amino acid sequence of the *E. coli* MurG protein.

58. The model of claim 52, wherein the MurG protein comprises an amino acid sequence that is at least about 60% identical to the amino acid sequence of the *E. coli* MurG protein.

59. The model of claim 52, wherein the MurG protein comprises an amino acid sequence selected, from the group consisting of the amino acid sequence of a MurG protein from *Escherichia coli, Bacillus subtilis, Aquefex aeolicus, Borrelia burgdorferi, Chlamydia pneumoniae, Chlamydia trachomatis, Enterococcus faecais, Enterococcus hirae, Haemophilus influenzae, Helicobacter pylori J99, Helicobacter pylori, Afycobacterium tuberculosis, Porphyromonas gingivalis, Rickettsia prowazekii, Streptomyces coeticolor, Streptomyces collinus, Streptococcus pneumoniae, Synechocystis* sp. (strain PCC6803), *Thermotoga maritime,* and *Treponema pallidum,* a mutant of any of the amino acid sequences, and a variants of any of the amino acid sequences.

60. The model of claim 52, wherein the MurG protein comprises an amino acid sequence selected from the group consisting of the amino acid sequences of MurG proteins as deposited in the NCBI database and identified with Accession Nos. CAB51993, A71316, E70579, C71699, F70195, A43727, JC1275, BVECMG, CEECAM, O83535, Q9ZK59, CAB85280, AAF39020, BAA18775, AAD26629, CAB73295, P37585, Q9ZHA9, Q9ZHDC0, Q9ZBA5, Q9X4H4, Q9WY74, P74657, O06224, Q9Z702, O84766, O69552, O67238, O51708, O25770, O07670, O07109, P45065, CAB66324, AAC68356, AAF06830, P18579, P17443, P17952, P16457, P07862, AAE23178, AAD53936, CAA18668, CAA38869, CAA38868, CAA38867, CAA38866, AAD08196, BAA01453, BAA01455, BAA01454, AAD19042, CAA45558, CAA74235, AAD10537, AAD06652, AAC95450, CAA14869, AAC73201, AAC65509, AAC67113, AAC45636, CAB08640, AAC22793, AAC07193, BAA24357, CAB13395, BAA01355, AAB35538, 1904153C, 1808265B, 1808265A, CAA36866, CAA36869, CAA36868, CAA36867, CAA36776, and AAA99436.

61. The model of claim 52, wherein the MurG protein comprises an amino acid sequence obtained from an organism selected from the group consisting of bacteria, small pathogenic organisms, cyano bacteria, higher-order bacteria, spirochetes and thermal stable bacteria.

62. The model of claim 52, wherein the MurG protein comprises an amino acid sequence obtained from an organism selected from the group consisting of *Escherichia coli, Bacillus subtilis, Aquefex aeolicus, Borrelia burgdorferi, Chlamydia*

pneumoniae, Chlamydia trachomatis, Enterococcus faecais, Enterococcus hirae, Haemophilus influenzae, Helicobacter pylori J99, Helicobacter pylori, Mycobacterium tuberculosis, Porphyromonas gingivalis, Rickettsia prowazekii,Streptomyces coelicolor, Streptomyces collinus, Streptococcus pneumoniae, Synechocystis sp. (strain PCC6803), *Thermotoga marithne,* and *Treponema pallidum.*

63. The model of claim 52, wherein the MurG protein is a structural homologue of the *E. coli* MurG protein.

64. The model of claim 52, wherein the structure comprises an n-terminal and C-terminal domain connected by a covalent peptide linker, and wherein each domain has an alpha/beta fold.

65. The model of claim 52, wherein the RMSD is less than 2.5 Å over at least 80 aligned C-alpha atoms in each domain.

66. The model of claim 52, wherein the N-terminal domain comprises two glycine rich loops.

67. The model of claim 66, wherein the, amino acid sequence of the two glycine rich loops comprises GGTGGH and G-GGYVSG.

68. The model of claim 52, wherein the C-terminal domain comprises one glycine rich loop.

69. The model of claim 68, wherein the glycine rich loop comprises the amino acid sequence GGSQGAR or GGS-GAR.

70. The model of claim 52, wherein the atomic coordinates are generated by the method comprising the steps of:

(a) providing a MurG protein in crystalline form;

(b) generating an electron-density map of the crystalline MurG protein; and

(c) analyzing the electron-density map to produce the atomic coordinates.

71. The model of claim 70, wherein the crystalline MurG protein is produced by a method comprising the steps of:

(a) combining MurG protein with UDP-GlcNAc; and

(b) inducing crystal formation to produce said crystalline MurG protein.

72. The model of claim 70, wherein the crystalline MurG protein is produced by the hanging drop method in which MurG in buffer is at a concentration of at least 5 ug/ml and is combined with a reservoir solution and crystallizes.

73. The model of claim 72, wherein the buffer has a pH range from about 6.5 to about 9.0, and a buffer concentration range from about 10 mM to about 200 mM.

74. The model of 73, wherein the buffer is a Tris or a Hepes buffer, having a pH from about 7.0 to about,8.5.

75. The model of 74, wherein the buffer has a pH of about 7.9.

76. The model of claim 73, wherein the buffer further comprises at least one salt, chelating agent, or reducing agent.

77. The model of claim 72, wherein the reservoir solution has a pH range from about 5.0 to about 9.0 and the buffer concentration ranges from about 10 mM to about 1M.

78. The model of claim 77, wherein the reservoir solution further comprises at least one suitable precipitant, a detergent, and a reducing agent.

79. The model of claim 78, wherein the reservoir solution comprises a NaMES or sodium citrate buffer having a pH from about 6.0 to about 7.0.

80. The model of claim 79, wherein the buffer has a p14 of about 6.5.

81. The model of claim 78, wherein the precipitant is selected from the group consisting of ammonium sulfate and sodium potassium tartrate.

82. The model of 78, wherein the detergent is TritonX-100.

83. The model of 78, wherein the reducing agent is DTT, DTE or beta-mercaptoethanol.

84. The model of claim 71, wherein the MurG protein and the UDP-GlcNAc are in a 1:3 molar ratio.

85. The model of claim 71, wherein the buffer comprises 0.1 M NaMES, pH6.5, 0.9M $(NH_4)_2SO_4$,0.4% TRITON X-100®, and 10 mM dithiothreitol (DTT).

86. The model of claim 71, wherein the step of generating an electron-density map comprises analyzing the crystalline MurG protein by X-ray diffraction.

87. The model of claim 70, wherein the model is a computer image generated by a computer-readable medium encoded with a set of three-dimensional coordinates of the three-dimensional structure, wherein, using a graphical display software program, the three-dimensional coordinates create an electronic file that can be

visualized on a computer capable of representing the electronic file as a three-dimensional image.

88. A model of a donor nucleotide binding site of a UDP-glycosyltransferase (MurG) protein, wherein the model represents a three-dimensional structure that substantially conforms to the atomic coordinates of Table 4.

89. The model of claim 88, wherein the donor nucleotide binding site is located within the MurG C-terminal domain.

90. The model of claim 88, wherein the structure substantially conforms to the atomic coordinates and B-values of Table 4.

91. The model of claim 88, wherein at least about 50% of the structure has an average root-mean-square (RMSD) of less than about 2.5Å for the conserved amino acid residues for the donor nucleotide binding site of the *E. coli* MurG.

92. The model of claim 88, wherein the donor nucleotide binding site comprises an amino acid sequence that is at least about 70% identical to the conserved amino acid residues of the donor nucleotide binding site of *E. coli* MurG.

93. The model of claim 88, wherein the donor nucleotide binding site comprises an amino acid sequence that is at least about 80% identical to the conserved amino acid residues of the donor nucleotide binding site of the *E. coli* MurG.

94. The model of claim 88, wherein the donor nucleotide binding site comprises an amino acid sequence that is at least about 90% identical to the conserved amino acid residues of the donor nucleotide binding site, of the *E. coli* MurG.

95. The model of claim 88, wherein the donor nucleotide binding site comprises an amino acid sequence that is at least about 95% identical to the conserved amino acid residues of the donor nucleotide binding site of the *E. coli* MurG.

96. The model of claim 88, wherein the atomic coordinates are generated by a method comprising the steps of:

(a) providing a MurG protein in a crystalline form:

(b) generating an electron-density map of said crystalline MurG protein; and

(c) analyzing the electron-density map to produce the atomic coordinates.

97. The model of claim 88, wherein the model is a computer image generated by a computer-readable medium encoded with a set of three-dimensional coordinates of the three-dimensional structure, wherein, using a graphical display

software program, the three-dimensional coordinates create an electronic file that can be visualized on a computer capable of representing the electronic file as a three-dimensional image.

98. A model of an acceptor binding site of a UDP-glycosyltransferase (MurG) protein, wherein the model represents a three-dimensional structure that substantially conforms to the atomic coordinates of Table 5.

99. The model of claim 98, wberein the structure substantially conforms to the atomic coordinates and B-values of Table 5.

100. The model of claim 98, wherein at least about 50% of the structure has an average root-mean-square (RMSD) of less than about 1.5Å for the conserved amino acid residues in the acceptor binding site.

101. The model of claim 98, wherein the acceptor binding site comprises an amino acid sequence that is at least about 70% identical to the conserved amino acid residues of the acceptor binding site of *E. coli* MurG.

102. The model of claim 98, wherein the acceptor binding site comprises an amino acid sequence that is at least about 80% identical to the conserved amino acid residues of the acceptor binding site of *E. coli* MurG.

103. The model of claim 98, wherein the acceptor binding site comprises an amino acid sequence that is at least about 90% identical to the conserved amino acid residues of the *E. coli* MurG.

104. The model of claim 98, wherein the acceptor binding site comprises an amino acid sequence that is at least about 95% identical to the conserved amino acid residues of the acceptor binding site of the *E. coli* MurG.

105. The model of claim 98, wherein the acceptor binding site comprises an amino acid sequence that is at least about 70% identical to the amino acid sequence selected from the group consisting of *Escherichia coli, Bacillus subtilis, Aquefex aeolicus, Borrelia burgdorferi, Chlamydia pneumoniae, Chlamydia trachomatis, Enterococcus faecais, Enterococcus hirae, Haemophilus influenzae, Helicobacter pylorl J99, Helicobacter pylori, Mycobacterium tuberculosis, Porphyromonas gingivalis, Rickettsia prowazekii,Streptomyces coelicolor, Streptomyces collinus, Streptococcus pneumoniae, Synechocystis* sp. (strain PCC6803), *Thermotoga maritime,* and *Treponema pallidum.*

106. The model of claim 98, wherein the atomic coordinates are generated by the method comprising the steps of:

(a) providing a MurG protein in a crystalline form:

(b) generating an electron-density map of said crystalline MurG protein; and

(c) analyzing the electron-density map to produce the atomic coordinates.

107. The model of claim 98, wherein the model is a computer image generated by a computer-readable medium encoded with a set of three-dimensional coordinates of the three-dimensional structure, wherein, using a graphical display software program, the three-dimensional coordinates create an electronic file that can be visualized on a computer capable of representing the electronic file as a three-dimensional image.

108. A model of a membrane association site of a UDP-glycosyltransferase (MurG) protein, wherein the model represents a three-dimensional structure that substantially conforms to the atomic coordinates of Table 6.

109. The model of claim 108, wherein the structure substantially conforms to the atomic coordinates and B-values of Table 4.

110. The model of claim 108, wherein at least about 50% of the structure has an average root-mean-square (RMSD) of less than about 1.5Å for conserved amino acid residues in the *E. coli* membrane association site.

111. The model of claim 108, wherein the membrane association site comprises an amino acid sequence that is at least about 70% identical to the conserved amino acid residues of the membrane association site of *E. coli* MurG.

112. The model of claim M, wherein the membrane association site comprises an amino acid sequence that is at least about 80% identical to the conserved amino acid residues of the membrane association site of the *E. coli* MurG.

113. The model of claim 108, wherein the membrane association site comprises an amino acid sequence that is at least about 90% identical to the conserved amino acid residues of the membrane association site of the *E. coli* MurG.

114. The model of claim 108, wherein the membrane association site comprises an amino acid sequence that is at least about 95% identical to the conserved amino acid residues of a membrane association site of the *E. coli* MurG.

115. The model of claim 108, wherein the membrane association site comprises an amino acid sequence that is at least about 70% identical to the amino acid sequence from organisms selected from the group consisting of *Escherichia coli, Bacillus subtilis, Aquefex aeolicus, Borrelia burgdorferi, Chlamydia pneumoniae, Chlamydia trachomatis, Enterococcus faecais, Enterococcus hirae, Haemophilus influenzae, Helicobacter pylori J99, Helicobacter pylori, Mycobacterium tuberculosis, Porphyromonas gingivalis, Rickettsia prowazekii, Streptomyces coelicolor, Streptomyces collinus, Streptococcus pneumoniae, Synechocystis* sp. (strain PCC6803), *Thermotoga maritime,* and *Treponema pallidum.*

116. The model of claim 108, wherein the model is a computer image generated by a computer-readable medium encoded with a set of three-dimensional coordinates of the three-dimensional structure, wherein, using a graphical display software program, the three-dimensional coordinates create an electronic file that can be visualized on a computer capable of representing the electronic file as a three-dimensional image.

117. A computer-assisted method of structure based drug design of bioactive compounds, comprising the steps of:

(a) providing a model of a UDP-glycosyltransferase (MurG) protein or a donor nucleotide binding site, acceptor binding site or membrane association site; and

(b) designing a chemical compound using said model.

118. The method of claim 117, further comprising the step of synthesizing the chemical compound.

119. The method of claim 118, further comprising the step of evaluating the bioactivity of the synthesized chemical compound.

120. The method of claim 118, wherein the model of the UDP-glycosyltransferase (MurG) protein represents a three-dimensional structure comprising the atomic coordinates listed in Table 1.

121. The method of claim 118, wherein the model of the donor nucleotide binding site represents a three-dimensional structure comprising the atomic coordinates Table 4.

122. The method of claim 118, wherein the model of the acceptor binding site represents a three-dimensional structure comprising the atomic coordinates in Table 5.

123. The method of claim 118, wherein the model of the membrane association site represent a three-dimensional structure comprising the atomic coordinates in Table 6.

124. The method of claim 118, wherein the model comprises a computer image generated when the atomic coordinates listed in Table 1 are analyzed on a computer using a graphical display software program to create an electronic file of the image and visualizing the electronic file on a computer capable of representing the electronic file as a three-dimensional image.

125. The method of claim 118, wherein the step of designing comprises computational screening of one or more databases of chemical compounds in which the three-dimensional structure of said compounds are known.

126. The method of claim 125, further comprising interacting a compound identified by the screening step with the model by computer.

127. The method of claim 118, wherein the step of designing comprises directed drug design.

128. The method of claim 118, wherein the step of designing comprises random drug design.

129. The method of claim 118, wherein the step of designing comprises grid-based drug design.

130. The method of claim 118, wherein the step of designing comprises selecting compounds which are predicted to mimic the three-dimensional structure of the three-dimensional structure of the MurG protein.

131. The method of claim 118, wherein the step of designing comprises selecting compounds which are predicted to bind to the three-dimensional structure of the MurG protein.

132. The method of claim 118, wherein the bioactivity is selected from the group consisting of inhibiting binding of a nucleotide donor compound to the MurG protein, inhibiting binding of an acceptor compound to the MurG protein, or inhibiting association of the MurG Protein to a membrane.

133. A model of the three-dimensional, structure of a MurG protein , wherein the model is produced by the following method comprising the steps of:

(a) providing an amino acid sequence of a MurG protein and the amino acid sequence of the *Escherichia coli* MurG protein;

(b) identifying structurally conserved regions shared between the MurG protein and the *E. coli* MurG protein; and

(c) determining atomic coordinates for the MurG protein by assigning the structurally conserved regions of the MurG protein to a three-dimensional structure using a three-dimensional structure of the MurG protein which substantially conforms to the atomic coordinates represented in Table 1, to derive a model of the three-dimensional structure of the MurG protein amino acid sequence.

134. The model of claim 133, wherein the MurG protein amino acid sequence comprises the sequence of an amino acid sequence selected from the group consisting of the amino acid sequences of MurG proteins as deposited in the NCBI database and identified with Accession Nos. CAB51993, A71316, E70579, C71699, F70195, A43727, JC1275, BVECMG, CEECAM, O83535, Q9ZK59, CAB85280, AAF39020, BAA18775, AAD26629, CAB73295, P37585, Q9ZHA9, Q9ZHDC0, Q9ZBA5, Q9X4H4, Q9WY74, P74657, O06224, Q9Z702, O84766, O69552, O67238, O51708, O25770, O07670, O07109, P45065, CAB66324, AAC68356, AAF06830, P18579, P17443, P17952, P16457, P07862, AAE23178, AAD53936, CAA18668, CAA38869, CAA38868, CAA38867, CAA38866, AAD08196, BAA01453, BAA01455, BAA01454, AAD19042, CAA45558, CAA74235, AAD10537, AAD06652, AAC95450, CAA14869, AAC73201, AAC65509, AAC67113, AAC45636, CAB08640, AAC22793, AAC07193, BAA24357, CAB13395, BAA01355, AAB35538, 1904153C, 1808265B, 1808265A, CAA36866, CAA36869, CAA36868, CAA36867, CAA36776, and AAA99436.

135. A composition for inhibiting the activity of a glycosyltransferase comprising a compound that inhibits the activity of a glycosyltransferase, wherein the compound is identified by the method comprising the steps of:

(a) providing a three-dimensional structure of a MurG protein;

(b) using the three-dimensional structure of the MurG protein to design a chemical compound that inhibits activity of a glycosyltransferase;

(c) synthesizing the chemical compound; and

(d) evaluating the ability of the chemical compound to inhibit the activity of a glycosyltransferase.

136. The composition of claim 135, wherein the glycosyltransferase is a MurG protein.

137. The composition of claim 135, wherein the three-dimensional structure of the MurG protein substantially conforms to atomic coordinates represented by Table 1.

138. The composition of claim 135, wherein the compound is selected from the group consisting of an inorganic and an organic compound.

139. The composition of claim 135, wherein the compound is a substituted pyrimidine analogs.

140. The composition, of claim 135, wherein the compound is selected from the group consisting of an analog of a MurG protein, a substrate analog of a MurG protein, a donor molecule analog of a MurG protein, and a membrane analog of a MurG protein.

141. The composition of claim 135, further comprising a component selected from the group consisting of an excipient an adjuvant, and a carrier.

142. A composition for stimulating the activity of a glycosyltransferase comprising a compound that stimulates the activity of a glycosyltransferase, wherein the compound is identified by the method comprising the steps of:

(a) providing a three-dimensional structure of a MurG protein;

(b) using the three-dimensional structure of the MurG protein to design a chemical compound that inhibits activity of a glycosyltransferase;

(c) synthesizing the chemical compound; and

(d) evaluating the ability of the chemical compound to stimulate the activity of a glycosyltransferase.

143. A method to determine a three-dimensional structure of a MurG protein comprising the steps of:

(a) providing an amino acid sequence of a MurG protein, wherein the three-dimensional structure of the MurG protein is not known;

(b) analyzing the pattern of folding of the amino acid sequence in a three-dimensional conformation by fold recognition; and

(c) comparing the pattern of folding of the MurG protein amino acid sequence with the three-dimensional structure of the *E. coli* MurG protein, wherein the three-dimensional structure of the *E. coli* MurG protein substantially conforms to the atomic coordinates represented in Table 1.

144. A method to derive a model of the three-dimensional structure of a MurG protein comprising the steps of:

(a) providing an amino acid sequence of a MurG protein;

(b) identifying structurally conserved regions shared between the MurG protein and the *E. coli* MurG protein;

(c) determining atomic coordinates for the MurG protein structure by assigning the structurally conserved regions of the MurG protein to a three-dimensional structure using a three-dimensional structure of the *E. coli* MurG protein based on atomic coordinates represented in Table 1 to derive a model of the three-dimensional structure of the MurG protein amino acid sequence.

145. The method of claim 144, further comprising assigning atomic coordinates for side chains of said MurG protein by determining sterically allowable positions using a library of rotamers.

146. A method to derive a three-dimensional structure of a crystallized MurG protein comprising the steps of:

(a) comparing the Patterson function of a crystallized MurG protein with the Patterson function of crystalline *E. coli* MurG protein to produce an electron-density map of the crystallized MurG protein; and

(b) analyzing the electron-density map to produce the three-dimensional structure of the crystallized MurG protein.

147. The method of claim 146, further comprising the step of rotating the Patterson function of the crystallized MurG protein on the Patterson function of the crystalline E coli MurG protein to determine the correct orientation of the crystallized MurG protein in a crystal of said crystallized MurG protein to identify the initial phases of the crystallized MurG protein.

148. The method of claim 146, further comprising the step of electronically stimulating the three-dimensional structure of the crystallized MurG protein to derive a computer image of the three-dimensional structure of the crystallized MurG protein.

ABSTRACT OF THE DISCLOSURE

The present invention relates to crystals of the *Escherichia coli* MurG, a membrane-associated UDP-glycosyltransferase involved in peptidoglycan biosynthesis. The present invention also relates to three-dimensional atomic coordinates of the MurG protein, three-dimensional structures of the protein, and images thereof. ~~The present invention also relates to the atomic coordinates and three-dimensional structures of the α-carbon backbone and of the α-carbon backbone and conserved amino acid residue sidechains of the MurG protein and images thereof. The present invention further relates to three-dimensional atomic coordinates of the donor nucleotide binding site, the acceptor binding site, and the membrane association site of the MurG protein, three-dimensional structures of the binding domains, and images thereof. The present invention also relates to computer readable media encoded with sets of the three-dimensional coordinates described herein.~~ The present invention relates to methods of crystallizing MurG proteins. ~~The present invention relates to models of three-dimensional structures of UDP-glycosyltransferases and, in particular, MurG proteins, based on the three-dimensional structure of crystals of the *Escherichia coli* MurG. The present invention also relates to models of the three-dimensional structures of the α-carbon backbone and the α-carbon backbone and conserved amino acid residue sidechains of UDP-glycosyltransferases and MurG proteins and of the binding sites thereof. The present invention also relates to methods of drug design using models of this invention, the compounds identified using models of the present invention that bind, inhibit or stimulate UDP-glycosyltransferases or MurG proteins, and compositions comprising compounds identified using the models of this invention for therapeutic or diagnositic uses. Also, the present invention relates to methods of making models of the present invention.~~